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Zwitterionic (*E*)-1-[(4-nitrophenyl)-iminiomethyl]naphthalen-2-olate

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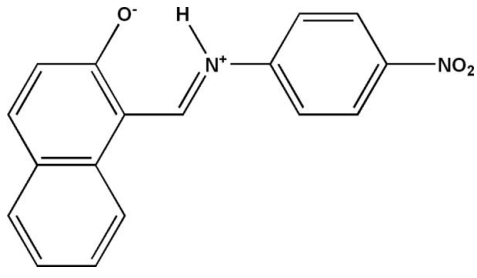
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.059; wR factor = 0.190; data-to-parameter ratio = 38.4.

The title compound, $C_{17}H_{12}N_2O_3$, was synthesized by the reaction of 2-hydroxy-1-naphthaldehyde with 4-nitrobenzenamine. These condense to form the Schiff base, which crystallizes in the zwitterionic form. In the structure, the keto–amino tautomer has a fairly short intramolecular N—H···O hydrogen bond between the 2-naphthalenone and amino groups, with electron delocalization. The molecule is essentially planar, with a dihedral angle of 1.96 (3)° between the ring systems. In the crystal, the molecules are linked *via* intermolecular C—H···O hydrogen bonds, forming a layer parallel to (101).

Related literature

For background to Schiff base compounds, see: Fan *et al.* (2007); Kim *et al.* (2005); Nimitsiriwat *et al.* (2004). For the pharmaceutical and medicinal activity of Schiff bases, see: Chen *et al.* (1997); Dao *et al.* (2000); Ren *et al.* (2002); Sriram *et al.* (2006); Karthikeyan *et al.* (2006). For Schiff bases in coordination chemistry, see: Ali *et al.* (2008); Kargar *et al.* (2009); Yeap *et al.* (2009). For related structures, see: Fun *et al.* (2009); Nadeem *et al.* (2009); Eltayeb *et al.* (2008). For standard bond lengths see: Allen, (2002).



Experimental

Crystal data

$C_{17}H_{12}N_2O_3$
M_r = 292.29
Monoclinic, $P2_1/c$
a = 8.0503 (6) Å
b = 12.8174 (9) Å
c = 13.1833 (10) Å
β = 97.271 (5)°
V = 1349.37 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.15 × 0.06 × 0.04 mm

Data collection

Bruker SMART CCD area-detector diffractometer
44074 measured reflections
7946 independent reflections
3658 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.190
S = 0.96
7946 reflections
207 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*N*···O3	1.09 (2)	1.57 (2)	2.5287 (15)	143 (2)
C5—H5···O2^{i}	0.93	2.59	3.5136 (16)	173
C16—H16···O2^{i}	0.93	2.53	3.4455 (17)	169

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2290).

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supplementary materials

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Zwitterionic (*E*)-1-[(4-nitrophenyl)iminiomethyl]naphthalen-2-olate

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Comment

Schiff base compounds have been widely investigated over a century (Fan *et al.*, 2007; Kim *et al.*, 2005; Nimitsiriwat *et al.*, 2004). Some of the compounds have been found to have pharmaceutical and medicinal fields (Chen *et al.*, 1997; Ren *et al.*, 2002; Dao *et al.*, 2000; Sriram *et al.*, 2006; Karthikeyan *et al.*, 2006). They are also used as versatile ligands in coordination chemistry (Ali *et al.*, 2008; Kargar *et al.*, 2009; Yeap *et al.*, 2009).

As part of our ongoing studies of Schiff base complexes and derivatives we report here synthesis and the crystal structure of the title compound, obtained by the reaction of 2-hydroxy-1-naphthaldehyde with 4-nitroaniline, which crystallized in a zwitterionic form with cationic iminium and anionic naphtholate group.

The molecular structure of (I), and the atomic numbering used, is illustrated in Fig. 1. All bond distances and angles are within the ranges of accepted values (CSD, Allen, 2002) and in literature (Fun *et al.*, 2009; Nadeem *et al.*, 2009; Eltayeb *et al.*, 2008).

The main molecule is essentially planar with an rms deviation of 0.0350 Å, and the crystal structure exhibit alternating layers parallel to (101) plane (Fig. 2). In the crystal, molecules are linked *via* intermolecular C—H···O hydrogen bonds to form a two-dimensional layers parallel to (101) (Table 1, Fig. 3) and additional stabilization within these layers is provided by N—O···π and π···π stacking interactions. These interaction bonds link the molecules within the layers and also link the layers together and reinforcing the cohesion of the structure. An intramolecular N—H···O hydrogen bond occurs.

Experimental

The title compound, (I), was prepared by refluxing a mixture of a solution containing (0.1 mmol) of 2-hydroxy-1-naphthaldehyde and (0.1 mmol) of 4-nitrobenzenamine in 20 ml methanol. The reaction mixture was stirred for 1 h under reflux. Microcrystals of (I) were obtained by allowing the clear solution to stand overnight. The powder product was dissolved and recrystallized from DMSO solution. Some red crystals were carefully isolated under polarizing microscope for analysis by x-ray diffraction.

Refinement

H7 and H2N were located in difference Fourier maps and refined isotropically. The remaining H atoms were localized on Fourier maps but introduced in calculated positions and treated as riding on their parent atoms (C_{aryl}) with C_{aryl}—H_{aryl}=0.95Å and $U_{iso}(H_{aryl})=1.2U_{eq}(C_{aryl})$.

Figures

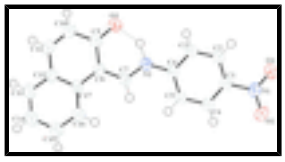

Fig. 1. (Farrugia, 1997) The asymmetric unit of the title compound with the atomic labeling scheme. Displacement are drawn at the 50% probability level. Hydrogen bond shown as dashed line.

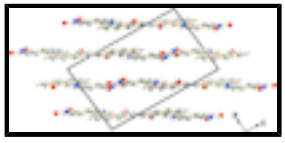

Fig. 2. (Brandenburg, 2001) A diagram of the layered crystal packing in (I), viewed down the *b* axis, showing layers parallel to (101).

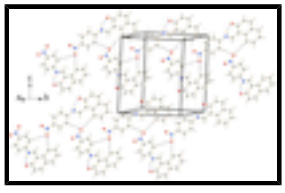

Fig. 3. (Brandenburg, 2001) A part of crystal packing of (I) showing hydrogen bond connections in the same layer as dashed line.

(*E*)-1-[(4-nitrophenyl)iminiomethyl]naphthalen-2-olate

Crystal data

$C_{17}H_{12}N_2O_3$	$F(000) = 608$
$M_r = 292.29$	$D_x = 1.439$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 5160 reflections
$a = 8.0503$ (6) Å	$\theta = 3.0$–$30.1°$
$b = 12.8174$ (9) Å	$\mu = 0.10$ mm^{-1}
$c = 13.1833$ (10) Å	$T = 296$ K
$\beta = 97.271$ (5)°	Needle, red
$V = 1349.37$ (17) Å^3	0.15 × 0.06 × 0.04 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	3658 reflections with $I > 2\sigma(I)$
Radiation source: sealed tube	$R_{int} = 0.074$
graphite	$\theta_{max} = 39.3°$, $\theta_{min} = 3.0°$
φ and ω scans	$h = -14 \rightarrow 12$
44074 measured reflections	$k = -20 \rightarrow 22$
7946 independent reflections	$l = -20 \rightarrow 23$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.059$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.190$	H atoms treated by a mixture of independent and constrained refinement
$S = 0.96$	$w = 1/[\sigma^2(F_o^2) + (0.0963P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
7946 reflections	$(\Delta/\sigma)_{max} = 0.001$
207 parameters	$\Delta\rho_{max} = 0.53$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.26$ 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}
O3	0.88419 (14)	−0.08384 (7)	0.31991 (8)	0.0392 (3)
O2	0.44266 (15)	−0.40551 (8)	0.79254 (8)	0.0426 (3)
O1	0.49601 (17)	−0.51766 (7)	0.67875 (9)	0.0500 (3)
N2	0.74356 (13)	−0.11314 (7)	0.47852 (8)	0.0264 (2)
N1	0.49499 (15)	−0.42784 (8)	0.71179 (9)	0.0320 (2)
C17	0.82974 (14)	0.16828 (9)	0.44636 (9)	0.0234 (2)
C8	0.82177 (14)	0.05641 (9)	0.42782 (9)	0.0234 (2)
C6	0.55083 (16)	−0.24287 (9)	0.68580 (10)	0.0274 (2)
H6	0.5057	−0.2275	0.7456	0.033*
C1	0.55862 (16)	−0.34487 (9)	0.65258 (10)	0.0259 (2)
C7	0.75161 (14)	−0.01080 (9)	0.49403 (10)	0.0245 (2)
C2	0.62367 (17)	−0.37057 (9)	0.56335 (10)	0.0300 (3)
H2	0.6267	−0.4396	0.5421	0.036*
C12	0.90181 (15)	0.23306 (9)	0.37664 (10)	0.0273 (2)
C16	0.76748 (16)	0.21715 (9)	0.52907 (10)	0.0293 (3)
H16	0.721	0.1766	0.5768	0.035*
C3	0.68369 (16)	−0.29201 (9)	0.50680 (10)	0.0290 (3)
H3	0.7278	−0.3079	0.4468	0.035*
C5	0.61127 (16)	−0.16388 (9)	0.62877 (10)	0.0265 (2)
H5	0.6069	−0.0949	0.6501	0.032*
C13	0.90891 (17)	0.34145 (10)	0.39091 (12)	0.0355 (3)
H13	0.9569	0.383	0.3446	0.043*
C10	0.96505 (18)	0.08390 (11)	0.27475 (11)	0.0352 (3)

H10	1.0122	0.0574	0.2193	0.042*
C4	0.67859 (14)	−0.18811 (9)	0.53937 (9)	0.0239 (2)
C9	0.88945 (16)	0.01310 (9)	0.34053 (10)	0.0280 (2)
C14	0.84615 (17)	0.38702 (10)	0.47216 (13)	0.0379 (3)
H14	0.8517	0.459	0.4812	0.045*
C15	0.77392 (17)	0.32417 (10)	0.54105 (12)	0.0346 (3)
H15	0.7296	0.3547	0.5957	0.041*
C11	0.96888 (17)	0.18704 (10)	0.29171 (11)	0.0336 (3)
H11	1.0168	0.2302	0.2467	0.04*
H7	0.704 (2)	0.0100 (13)	0.5544 (14)	0.043 (5)*
H2N	0.798 (3)	−0.1327 (18)	0.4091 (18)	0.080 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0597 (6)	0.0256 (4)	0.0362 (5)	−0.0031 (4)	0.0217 (5)	−0.0042 (4)
O2	0.0637 (7)	0.0342 (5)	0.0348 (5)	−0.0030 (5)	0.0249 (5)	0.0036 (4)
O1	0.0847 (9)	0.0207 (4)	0.0502 (7)	−0.0069 (5)	0.0308 (6)	0.0002 (4)
N2	0.0325 (5)	0.0198 (4)	0.0283 (5)	−0.0011 (4)	0.0097 (4)	0.0016 (4)
N1	0.0419 (6)	0.0241 (5)	0.0322 (6)	−0.0016 (4)	0.0134 (5)	0.0031 (4)
C17	0.0224 (5)	0.0216 (5)	0.0260 (6)	−0.0003 (4)	0.0023 (4)	0.0025 (4)
C8	0.0253 (5)	0.0215 (5)	0.0235 (5)	−0.0003 (4)	0.0044 (4)	0.0014 (4)
C6	0.0332 (6)	0.0226 (5)	0.0282 (6)	−0.0006 (4)	0.0111 (5)	−0.0012 (4)
C1	0.0320 (6)	0.0206 (4)	0.0264 (6)	−0.0007 (4)	0.0089 (5)	0.0015 (4)
C7	0.0256 (5)	0.0212 (5)	0.0271 (6)	−0.0002 (4)	0.0052 (4)	0.0017 (4)
C2	0.0395 (7)	0.0196 (5)	0.0335 (6)	0.0000 (4)	0.0148 (5)	−0.0022 (4)
C12	0.0257 (5)	0.0236 (5)	0.0329 (6)	−0.0022 (4)	0.0054 (5)	0.0037 (4)
C16	0.0334 (6)	0.0251 (5)	0.0302 (6)	−0.0001 (5)	0.0073 (5)	−0.0012 (4)
C3	0.0369 (6)	0.0222 (5)	0.0306 (6)	−0.0001 (4)	0.0151 (5)	−0.0018 (4)
C5	0.0326 (6)	0.0193 (4)	0.0290 (6)	−0.0019 (4)	0.0097 (5)	−0.0026 (4)
C13	0.0334 (6)	0.0245 (5)	0.0499 (9)	−0.0044 (5)	0.0108 (6)	0.0053 (5)
C10	0.0471 (8)	0.0325 (6)	0.0291 (6)	−0.0030 (5)	0.0164 (6)	0.0009 (5)
C4	0.0268 (5)	0.0201 (4)	0.0259 (6)	−0.0012 (4)	0.0075 (4)	0.0005 (4)
C9	0.0334 (6)	0.0257 (5)	0.0259 (6)	−0.0012 (4)	0.0076 (5)	−0.0006 (4)
C14	0.0357 (7)	0.0220 (5)	0.0565 (9)	−0.0029 (5)	0.0079 (7)	−0.0021 (6)
C15	0.0367 (7)	0.0260 (6)	0.0413 (8)	0.0011 (5)	0.0059 (6)	−0.0060 (5)
C11	0.0382 (7)	0.0319 (6)	0.0329 (7)	−0.0054 (5)	0.0129 (6)	0.0046 (5)

Geometric parameters (Å, °)

O3—C9	1.2714 (15)	C2—H2	0.93
O2—N1	1.2274 (14)	C12—C13	1.4021 (17)
O1—N1	1.2312 (14)	C12—C11	1.4304 (18)
N2—C7	1.3279 (15)	C16—C15	1.3810 (17)
N2—C4	1.3951 (14)	C16—H16	0.93
N2—H2N	1.09 (2)	C3—C4	1.4015 (16)
N1—C1	1.4504 (14)	C3—H3	0.93
C17—C16	1.4039 (16)	C5—C4	1.3931 (16)
C17—C12	1.4163 (15)	C5—H5	0.93

C17—C8	1.4546 (16)	C13—C14	1.372 (2)
C8—C7	1.3957 (15)	C13—H13	0.93
C8—C9	1.4450 (16)	C10—C11	1.3405 (18)
C6—C1	1.3827 (17)	C10—C9	1.4421 (17)
C6—C5	1.3855 (16)	C10—H10	0.93
C6—H6	0.93	C14—C15	1.395 (2)
C1—C2	1.3866 (16)	C14—H14	0.93
C7—H7	0.962 (19)	C15—H15	0.93
C2—C3	1.3763 (16)	C11—H11	0.93
C7—N2—C4	127.33 (10)	C17—C16—H16	119.3
C7—N2—H2N	109.9 (12)	C2—C3—C4	120.22 (11)
C4—N2—H2N	122.8 (12)	C2—C3—H3	119.9
O2—N1—O1	122.91 (11)	C4—C3—H3	119.9
O2—N1—C1	118.62 (10)	C6—C5—C4	119.81 (10)
O1—N1—C1	118.47 (10)	C6—C5—H5	120.1
C16—C17—C12	117.28 (11)	C4—C5—H5	120.1
C16—C17—C8	123.91 (10)	C14—C13—C12	120.93 (12)
C12—C17—C8	118.81 (10)	C14—C13—H13	119.5
C7—C8—C9	118.96 (10)	C12—C13—H13	119.5
C7—C8—C17	121.07 (10)	C11—C10—C9	121.53 (12)
C9—C8—C17	119.96 (10)	C11—C10—H10	119.2
C1—C6—C5	119.07 (10)	C9—C10—H10	119.2
C1—C6—H6	120.5	C5—C4—N2	123.17 (10)
C5—C6—H6	120.5	C5—C4—C3	120.04 (10)
C6—C1—C2	122.04 (11)	N2—C4—C3	116.79 (10)
C6—C1—N1	119.32 (10)	O3—C9—C10	119.44 (11)
C2—C1—N1	118.64 (10)	O3—C9—C8	122.68 (11)
N2—C7—C8	121.95 (11)	C10—C9—C8	117.87 (11)
N2—C7—H7	112.6 (10)	C13—C14—C15	119.19 (12)
C8—C7—H7	125.4 (10)	C13—C14—H14	120.4
C3—C2—C1	118.81 (11)	C15—C14—H14	120.4
C3—C2—H2	120.6	C16—C15—C14	120.79 (12)
C1—C2—H2	120.6	C16—C15—H15	119.6
C13—C12—C17	120.46 (11)	C14—C15—H15	119.6
C13—C12—C11	120.03 (11)	C10—C11—C12	122.29 (11)
C17—C12—C11	119.50 (11)	C10—C11—H11	118.9
C15—C16—C17	121.34 (11)	C12—C11—H11	118.9
C15—C16—H16	119.3		
C16—C17—C8—C7	−0.89 (19)	C1—C6—C5—C4	0.0 (2)
C12—C17—C8—C7	−179.83 (12)	C17—C12—C13—C14	−0.2 (2)
C16—C17—C8—C9	−179.95 (12)	C11—C12—C13—C14	−179.64 (14)
C12—C17—C8—C9	1.11 (18)	C6—C5—C4—N2	−179.26 (12)
C5—C6—C1—C2	−0.6 (2)	C6—C5—C4—C3	0.6 (2)
C5—C6—C1—N1	−179.78 (12)	C7—N2—C4—C5	−0.3 (2)
O2—N1—C1—C6	−3.2 (2)	C7—N2—C4—C3	179.85 (12)
O1—N1—C1—C6	176.80 (13)	C2—C3—C4—C5	−0.6 (2)
O2—N1—C1—C2	177.56 (13)	C2—C3—C4—N2	179.28 (12)
O1—N1—C1—C2	−2.4 (2)	C11—C10—C9—O3	177.94 (14)

C4—N2—C7—C8	179.22 (12)	C11—C10—C9—C8	−1.8 (2)
C9—C8—C7—N2	−0.77 (19)	C7—C8—C9—O3	1.8 (2)
C17—C8—C7—N2	−179.84 (11)	C17—C8—C9—O3	−179.16 (12)
C6—C1—C2—C3	0.6 (2)	C7—C8—C9—C10	−178.46 (12)
N1—C1—C2—C3	179.80 (12)	C17—C8—C9—C10	0.62 (19)
C16—C17—C12—C13	−0.20 (19)	C12—C13—C14—C15	−0.2 (2)
C8—C17—C12—C13	178.81 (12)	C17—C16—C15—C14	−1.4 (2)
C16—C17—C12—C11	179.27 (12)	C13—C14—C15—C16	1.0 (2)
C8—C17—C12—C11	−1.71 (18)	C9—C10—C11—C12	1.3 (2)
C12—C17—C16—C15	0.98 (19)	C13—C12—C11—C10	−179.98 (14)
C8—C17—C16—C15	−177.98 (13)	C17—C12—C11—C10	0.5 (2)
C1—C2—C3—C4	0.0 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2N···O3	1.09 (2)	1.57 (2)	2.5287 (15)	143 (2)
C5—H5···O2^{i}	0.93	2.59	3.5136 (16)	173
C16—H16···O2^{i}	0.93	2.53	3.4455 (17)	169

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

Fig. 1

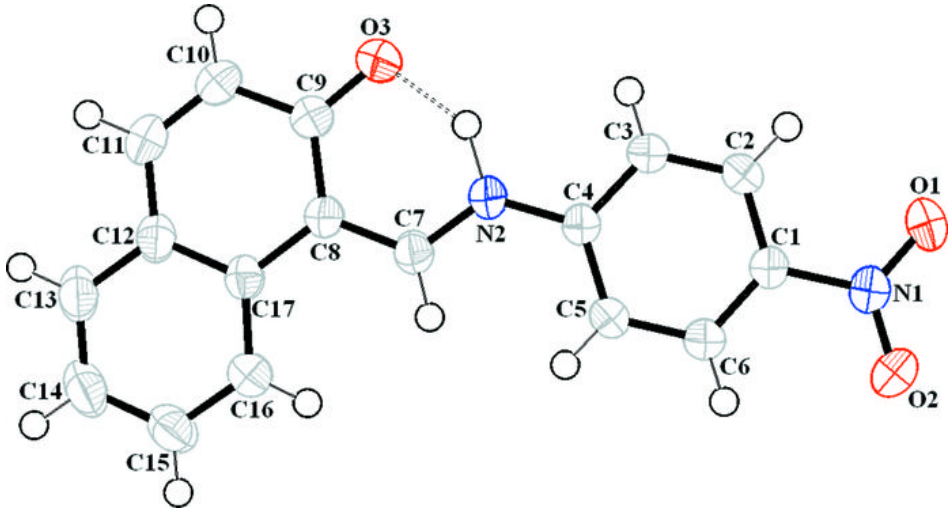
O3
C10
C9
C11
C3
C2
O1
C4
C12
C7
N2
C8
C1
C13
C17
C5
N1
C14
C16
C6
O2
C15

Fig. 2

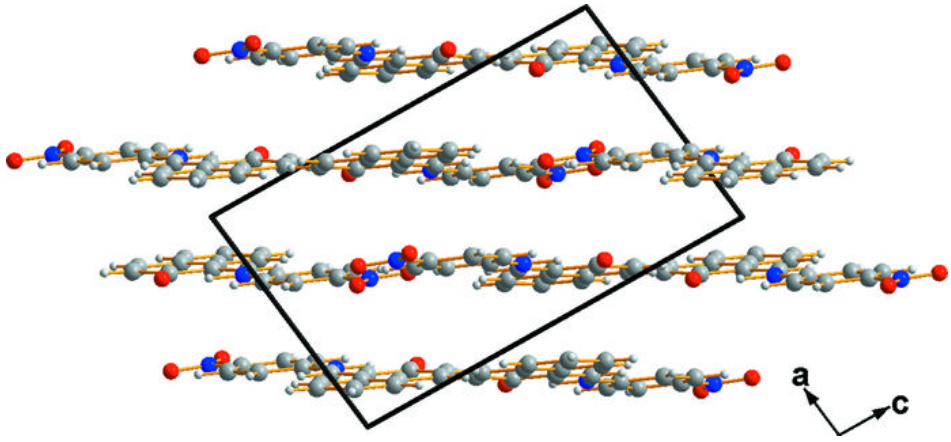

Fig. 3