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3-(3-Methoxyanilino)isobenzofuran-1(3*H*)-one[1]

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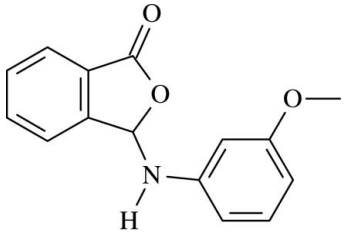
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.025; wR factor = 0.063; data-to-parameter ratio = 6.9.

The crystal structure of the title compound, $C_{15}H_{13}NO_3$, is stabilized by inversion-related N—H···O and C—H···O intermolecular hydrogen bonds and C—H···π interactions. The N—H···O hydrogen bonds generate two $C(6)$ chains, one within the other, and these chains are linked by C—H···O intermolecular hydrogen bonds forming $R_4^4(21)$ ring motifs. The phthalide part of the molecule is planar, and the dihedral angle between the phthalide group and the other benzene ring is 62.81 (8)°.

Related literature

For related structures, see: Büyükgüngör & Odabaşoğlu, (2006*a*,*b*); Odabaşoğlu & Büyükgüngör (2006*a*–*r*; 2007*a*,*b*,*c*). For related literature, see: Aoki *et al.* (1973); Büyükgüngör & Odabaşoğlu (2007); Etter (1990); Lacova (1973); Elderfield (1951); Tsi & Tan (1997); Bellasio (1974); Roy & Sarkar (2005).



Experimental

Crystal data

$C_{15}H_{13}NO_3$
M_r = 255.26
Monoclinic, *Cc*
a = 9.8103 (13) Å
b = 23.541 (3) Å
c = 7.2590 (10) Å
β = 130.756 (9)°
V = 1269.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.72 × 0.47 × 0.15 mm

Data collection

Stoe IPDS-2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.954, T_{max} = 0.987
6073 measured reflections
1227 independent reflections
1154 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.063
S = 1.07
1227 reflections
177 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.09 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.87 (2)	2.15 (3)	3.005 (2)	165.7 (19)
C4—H4···O2^{ii}	0.93	2.58	3.394 (3)	146
C12—H12···*Cg*1^{iii}	0.93	2.77	3.594 (3)	148

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); 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: AT2418).

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[1] 3-Substituted phthalides. Part XXVI.

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supplementary materials

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3-(3-Methoxyanilino)isobenzofuran-1(3*H*)-one

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Comment

Phthalides (isobenzofuranones) have important biological activities (Aoki *et al.*, 1973; Lacova, 1973; Elderfield, 1951; Tsi & Tan, 1997; Bellasio, 1974; Roy & Sarkar, 2005). As part of a continuing study of the interplay between molecular conformation and supramolecular aggregation in 3-substituted phthalides, we now report the structure of the title compound, 3-(3-methoxyphenylamino)isobenzofuran-1(3*H*)-one, (I) (Fig. 1).

The geometry of the molecule of (I) does not show any significant differences from the average geometry found for 2- and 3-metoxy isomers (Odabaşoğlu & Büyükgüngör, 2006*b*,c) and other isobenzofuran-1(3*H*)-ones (Büyükgüngör & Odabaşoğlu, 2006*a*,b, 2007; Odabaşoğlu & Büyükgüngör, 2006*a*,b,c,d,e,f,g,h,i,j,k,l,m,n,o,p,q,r; Odabaşoğlu & Büyükgüngör, 2007*a*,b,c). The phthalide group (C1—C8/O2) is planar, the largest deviation from the mean plane being −0.021 (2) Å for atom C8. The dihedral angle between the mean planes of the phthalide group and the phenyl ring is 62.81 (8) °.

In (I), the crystal packing is stabilized by, N—H···O, C—H···O intermolecular hydrogen bonds and C—H···π interactions (Fig. 2, Table 1). The N—H···O hydrogen bonds generate two C(6) chains one within the other and these chains are linked by C—H···O intermolecular hydrogen bonds forming $R_4^4(21)$ ring motifs (Fig.3) (Etter, 1990). The C12—H12···*Cg*1 (*Cg*1 is the centroid of the C9—C14 ring) interaction parameters are given in Table 1.

Experimental

The title compound was prepared according to the method described by Odabaşoğlu & Büyükgüngör (2006*a*), using phthalaldehydic acid and 3-methoxylaniline as starting materials (yield 90%; m.p. 428–429 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol (95%) solution at room temperature.

Refinement

All C-bound H atoms were refined using the riding model approximation with d(C—H) = 0.93 for aromatic, d(C—H) = 0.98 for methine and d(C—H) = 0.96 for methyl [U_{iso}(H) = 1.2 or 1.5U_{eq}(parent atom)]. N-bound H atom was located in Fourier difference map and refined freely due to its taking part in H-bond. The absolute structure could not be determined, and 1110 Friedel pairs were averaged before the last refinement.

Figures

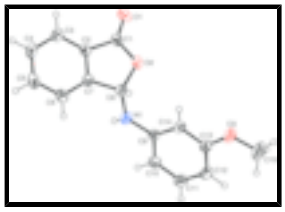

Fig. 1. A view of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

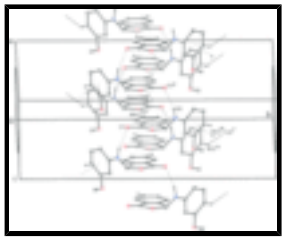

Fig. 2. Part of the crystal structure of (I), showing the formation of one within the other two c6 chains [Symmetry codes: (i) $x-1, -y+1, 1/2-z$; (ii) $x, 1-y, z-1/2$; (iii) $1-x, y, z-1/2$; (iv) $1-x, y, -z$; (v) $x-1/2, 3/2-y, z-1/2$].

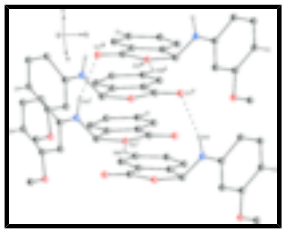

Fig. 3. Part of the crystal structure of (I), showing the holes along the *x* axis·[Symmetry codes: (i) $x-1, 1-y, z-1/2$; (ii) $x, 1-y, z+1/2$; (iii) $x-1, y, z$].

3-(3-Methoxyanilino)isobenzofuran-1(3*H*)-one

Crystal data

$C_{15}H_{13}NO_3$	F_{000} = 536
M_r = 255.26	D_x = 1.335 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C -2yc	Cell parameters from 6073 reflections
a = 9.8103 (13) Å	θ = 2.9–27.3º
b = 23.541 (3) Å	μ = 0.09 mm^{-1}
c = 7.2590 (10) Å	*T* = 296 K
β = 130.756 (9)º	Prismatic plate, colourless
V = 1269.9 (3) Å^3	0.72 × 0.47 × 0.15 mm
Z = 4	

Data collection

Stoe IPDS-2 diffractometer	1227 independent reflections
Monochromator: plane graphite	1154 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	R_{int} = 0.029
T = 296 K	θ_{max} = 26.0º
ω scans	θ_{min} = 2.9º
Absorption correction: integration	*h* = −12→11

(X-RED32; Stoe & Cie, 2002)

T_{min} = 0.954, T_{max} = 0.987

6073 measured reflections

k = −28→28

l = −8→8

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.025

$wR(F^2)$ = 0.063

S = 1.07

1227 reflections

177 parameters

2 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 0.1156P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.16 e Å^{-3}

$\Delta\rho_{min}$ = −0.08 e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0125 (17)

Absolute structure: Flack (1983), 1110 Friedel pairs

Flack parameter: ?

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}
C1	0.5126 (3)	0.47569 (8)	0.2907 (3)	0.0423 (4)
C2	0.3358 (2)	0.49461 (7)	0.1978 (3)	0.0389 (4)
C3	0.1898 (3)	0.46323 (8)	0.1291 (3)	0.0477 (4)
H3	0.1935	0.4238	0.1354	0.057*
C4	0.0393 (3)	0.49238 (10)	0.0514 (4)	0.0558 (5)
H4	−0.0609	0.4724	0.0040	0.067*
C5	0.0344 (3)	0.55134 (10)	0.0424 (4)	0.0569 (5)
H5	−0.0683	0.5702	−0.0077	0.068*
C6	0.1793 (3)	0.58260 (9)	0.1066 (4)	0.0508 (5)
H6	0.1748	0.6220	0.0970	0.061*
C7	0.3302 (2)	0.55322 (7)	0.1852 (3)	0.0394 (4)

C8	0.5047 (2)	0.57507 (8)	0.2636 (3)	0.0420 (4)
H8	0.4831	0.5933	0.1253	0.050*
C9	0.7376 (3)	0.64688 (7)	0.5373 (3)	0.0399 (4)
C10	0.8079 (3)	0.68262 (8)	0.7342 (3)	0.0478 (4)
H10	0.7604	0.6823	0.8108	0.057*
C11	0.9473 (3)	0.71831 (8)	0.8144 (4)	0.0553 (5)
H11	0.9915	0.7428	0.9432	0.066*
C12	1.0243 (3)	0.71886 (8)	0.7084 (4)	0.0559 (5)
H12	1.1196	0.7431	0.7655	0.067*
C13	0.9560 (3)	0.68262 (7)	0.5161 (4)	0.0478 (4)
C14	0.8121 (3)	0.64691 (7)	0.4281 (3)	0.0436 (4)
H14	0.7661	0.6232	0.2966	0.052*
C15	1.1826 (5)	0.70784 (16)	0.4999 (7)	0.0928 (10)
H15A	1.1666	0.7477	0.5090	0.111*
H15B	1.2134	0.7022	0.4001	0.111*
H15C	1.2774	0.6935	0.6603	0.111*
N1	0.5904 (2)	0.61331 (7)	0.4565 (3)	0.0483 (4)
O1	0.5718 (2)	0.42796 (6)	0.3314 (3)	0.0554 (4)
O2	0.61074 (18)	0.52137 (5)	0.3283 (2)	0.0479 (3)
O3	1.0211 (2)	0.67872 (7)	0.3974 (3)	0.0660 (4)
H1	0.577 (3)	0.6073 (9)	0.563 (5)	0.053 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0418 (11)	0.0481 (10)	0.0414 (9)	0.0018 (8)	0.0291 (9)	−0.0004 (7)
C2	0.0375 (10)	0.0433 (9)	0.0354 (8)	0.0002 (7)	0.0236 (8)	−0.0010 (7)
C3	0.0446 (12)	0.0512 (10)	0.0453 (9)	−0.0092 (9)	0.0285 (9)	−0.0048 (8)
C4	0.0360 (12)	0.0766 (13)	0.0497 (10)	−0.0106 (10)	0.0257 (10)	−0.0027 (11)
C5	0.0348 (12)	0.0795 (14)	0.0515 (11)	0.0112 (11)	0.0260 (10)	0.0085 (11)
C6	0.0448 (12)	0.0515 (10)	0.0524 (10)	0.0112 (9)	0.0301 (10)	0.0074 (9)
C7	0.0360 (10)	0.0439 (9)	0.0365 (8)	−0.0002 (7)	0.0229 (8)	0.0012 (7)
C8	0.0399 (11)	0.0434 (9)	0.0448 (10)	−0.0015 (8)	0.0286 (9)	0.0008 (7)
C9	0.0390 (10)	0.0337 (8)	0.0423 (9)	0.0010 (7)	0.0244 (8)	0.0034 (6)
C10	0.0485 (12)	0.0457 (10)	0.0497 (10)	0.0024 (8)	0.0323 (10)	−0.0014 (8)
C11	0.0564 (14)	0.0456 (10)	0.0541 (11)	−0.0076 (9)	0.0318 (11)	−0.0124 (8)
C12	0.0514 (13)	0.0453 (10)	0.0655 (13)	−0.0125 (9)	0.0357 (11)	−0.0077 (9)
C13	0.0505 (13)	0.0389 (9)	0.0565 (10)	−0.0031 (8)	0.0360 (10)	0.0017 (8)
C14	0.0461 (11)	0.0365 (8)	0.0463 (9)	−0.0043 (8)	0.0294 (9)	−0.0016 (7)
C15	0.092 (2)	0.110 (2)	0.110 (2)	−0.0432 (18)	0.081 (2)	−0.0240 (18)
N1	0.0511 (11)	0.0514 (9)	0.0492 (9)	−0.0107 (7)	0.0357 (9)	−0.0053 (7)
O1	0.0625 (10)	0.0496 (8)	0.0628 (8)	0.0147 (7)	0.0446 (8)	0.0058 (6)
O2	0.0371 (8)	0.0516 (8)	0.0577 (8)	0.0003 (6)	0.0321 (7)	−0.0014 (6)
O3	0.0706 (11)	0.0706 (10)	0.0785 (10)	−0.0232 (8)	0.0582 (10)	−0.0140 (8)

Geometric parameters (Å, °)

C1—O1	1.209 (2)	C9—C14	1.386 (3)
C1—O2	1.347 (2)	C9—C10	1.393 (3)

C1—C2	1.461 (3)	C9—N1	1.395 (2)
C2—C7	1.382 (2)	C10—C11	1.370 (3)
C2—C3	1.383 (3)	C10—H10	0.9300
C3—C4	1.371 (3)	C11—C12	1.386 (3)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.389 (3)	C12—C13	1.380 (3)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.383 (3)	C13—O3	1.370 (2)
C5—H5	0.9300	C13—C14	1.389 (3)
C6—C7	1.376 (3)	C14—H14	0.9300
C6—H6	0.9300	C15—O3	1.412 (3)
C7—C8	1.499 (3)	C15—H15A	0.9600
C8—N1	1.393 (2)	C15—H15B	0.9600
C8—O2	1.504 (2)	C15—H15C	0.9600
C8—H8	0.9800	N1—H1	0.87 (2)
O1—C1—O2	121.77 (19)	C14—C9—N1	123.20 (16)
O1—C1—C2	129.19 (19)	C10—C9—N1	117.19 (16)
O2—C1—C2	109.04 (15)	C11—C10—C9	119.68 (18)
C7—C2—C3	121.50 (18)	C11—C10—H10	120.2
C7—C2—C1	108.59 (16)	C9—C10—H10	120.2
C3—C2—C1	129.91 (17)	C10—C11—C12	121.65 (19)
C4—C3—C2	117.66 (18)	C10—C11—H11	119.2
C4—C3—H3	121.2	C12—C11—H11	119.2
C2—C3—H3	121.2	C13—C12—C11	118.34 (19)
C3—C4—C5	120.98 (19)	C13—C12—H12	120.8
C3—C4—H4	119.5	C11—C12—H12	120.8
C5—C4—H4	119.5	O3—C13—C12	124.01 (18)
C6—C5—C4	121.27 (19)	O3—C13—C14	114.89 (17)
C6—C5—H5	119.4	C12—C13—C14	121.10 (18)
C4—C5—H5	119.4	C9—C14—C13	119.62 (16)
C7—C6—C5	117.58 (19)	C9—C14—H14	120.2
C7—C6—H6	121.2	C13—C14—H14	120.2
C5—C6—H6	121.2	O3—C15—H15A	109.5
C6—C7—C2	120.99 (18)	O3—C15—H15B	109.5
C6—C7—C8	129.64 (18)	H15A—C15—H15B	109.5
C2—C7—C8	109.37 (16)	O3—C15—H15C	109.5
N1—C8—C7	113.20 (16)	H15A—C15—H15C	109.5
N1—C8—O2	112.88 (15)	H15B—C15—H15C	109.5
C7—C8—O2	102.45 (14)	C8—N1—C9	124.63 (16)
N1—C8—H8	109.4	C8—N1—H1	116.3 (15)
C7—C8—H8	109.4	C9—N1—H1	115.4 (15)
O2—C8—H8	109.4	C1—O2—C8	110.52 (14)
C14—C9—C10	119.60 (17)	C13—O3—C15	117.35 (19)
O1—C1—C2—C7	178.91 (18)	N1—C9—C10—C11	−177.19 (18)
O2—C1—C2—C7	−1.37 (19)	C9—C10—C11—C12	−1.7 (3)
O1—C1—C2—C3	−1.1 (3)	C10—C11—C12—C13	0.6 (3)
O2—C1—C2—C3	178.65 (17)	C11—C12—C13—O3	−179.4 (2)
C7—C2—C3—C4	−1.1 (3)	C11—C12—C13—C14	0.8 (3)

C1—C2—C3—C4	178.88 (18)	C10—C9—C14—C13	0.0 (3)
C2—C3—C4—C5	0.0 (3)	N1—C9—C14—C13	178.47 (18)
C3—C4—C5—C6	1.4 (3)	O3—C13—C14—C9	179.10 (18)
C4—C5—C6—C7	−1.5 (3)	C12—C13—C14—C9	−1.1 (3)
C5—C6—C7—C2	0.4 (3)	C7—C8—N1—C9	−168.78 (16)
C5—C6—C7—C8	179.40 (18)	O2—C8—N1—C9	75.4 (2)
C3—C2—C7—C6	0.9 (3)	C14—C9—N1—C8	1.9 (3)
C1—C2—C7—C6	−179.03 (16)	C10—C9—N1—C8	−179.54 (18)
C3—C2—C7—C8	−178.27 (15)	O1—C1—O2—C8	−179.84 (17)
C1—C2—C7—C8	1.8 (2)	C2—C1—O2—C8	0.41 (17)
C6—C7—C8—N1	57.6 (3)	N1—C8—O2—C1	122.68 (16)
C2—C7—C8—N1	−123.30 (16)	C7—C8—O2—C1	0.60 (17)
C6—C7—C8—O2	179.43 (18)	C12—C13—O3—C15	9.0 (4)
C2—C7—C8—O2	−1.45 (18)	C14—C13—O3—C15	−171.2 (2)
C14—C9—C10—C11	1.4 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.87 (2)	2.15 (3)	3.005 (2)	165.7 (19)
C4—H4···O2^{ii}	0.93	2.58	3.394 (3)	146
C12—H12···Cg1^{iii}	0.93	2.77	3.594 (3)	148

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

Fig. 1

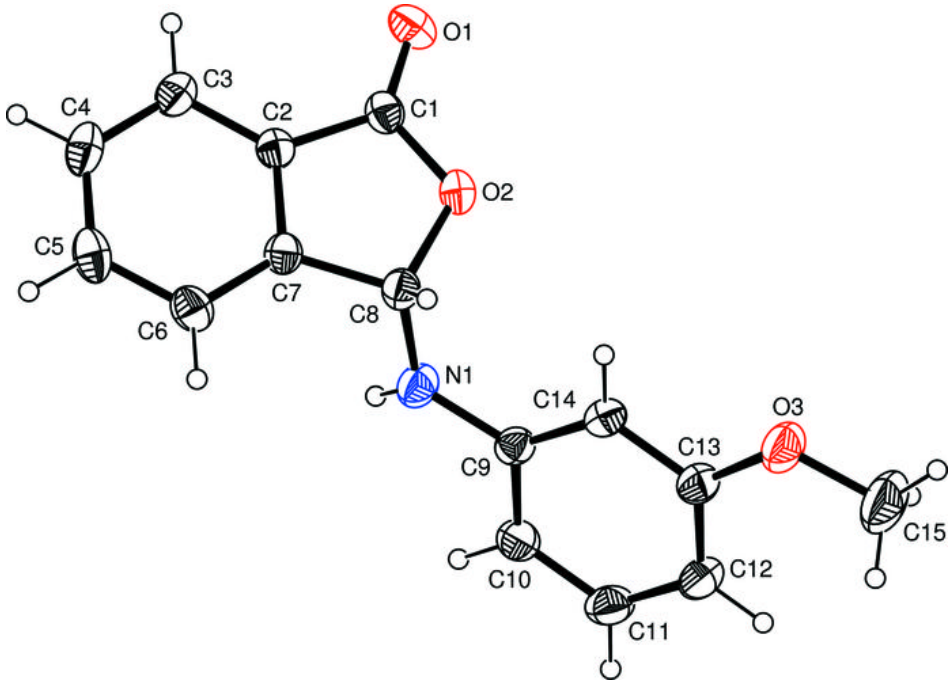

Fig. 2

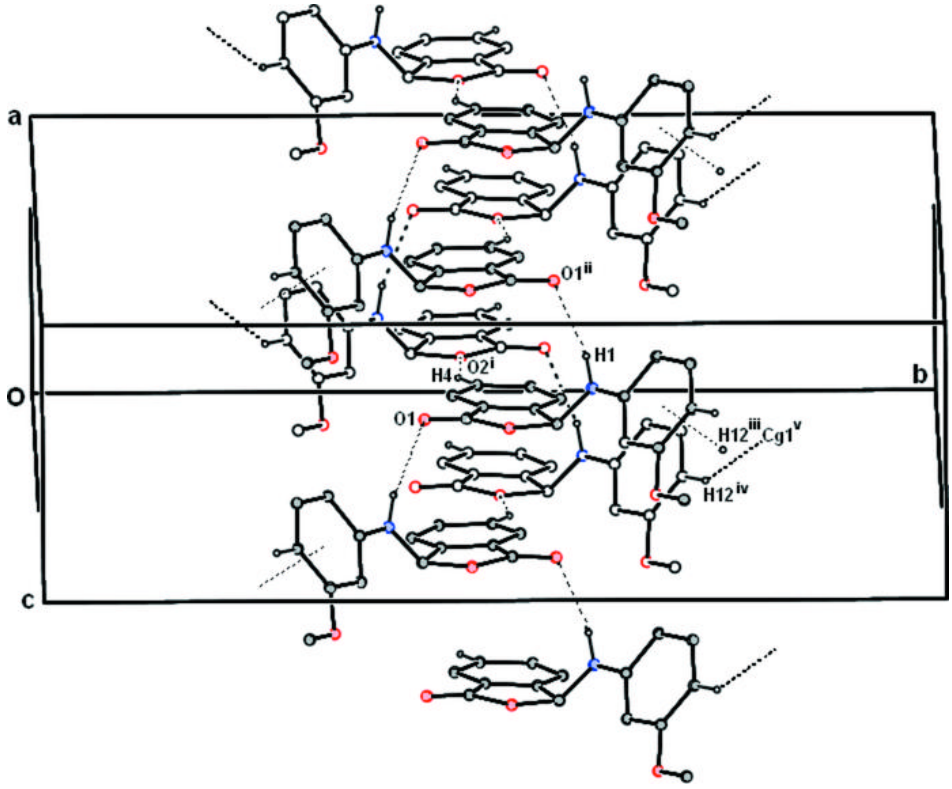

Fig. 3