Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(6-Methyl-2-pyridylamino)isobenzofuran-1(3*H*)-one[1]

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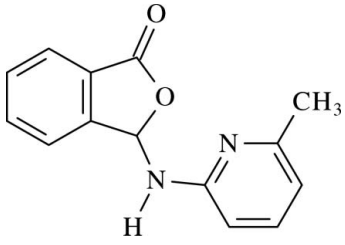
Received 3 October 2007; accepted 10 October 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.095; data-to-parameter ratio = 11.5.

The crystal structure of the title compound, $C_{14}H_{12}N_2O_2$, is stabilized by intermolecular N—H···O and C—H···N hydrogen bonds and also by C—H···π and π–π [centroid–centroid distance 3.822 (1) Å and a plane-to-plane separation 3.697 Å] interactions. The N—H···O and C—H···N hydrogen bonds generate edge-fused $R_2^1(6)R_4^4(24)R_2^1(6)$ ring motifs. The phthalide group is planar and oriented with respect to the pyridine ring at a dihedral angle of 83.21 (9)°.

Related literature

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



Experimental

Crystal data

$C_{14}H_{12}N_2O_2$
M_r = 240.26
Orthorhombic, *Pbca*
a = 10.1367 (7) Å
b = 22.519 (2) Å
c = 10.8253 (8) Å
V = 2471.0 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.64 × 0.36 × 0.14 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.970, T_{max} = 0.990
17021 measured reflections
2437 independent reflections
1265 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.095
S = 0.89
2437 reflections
212 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.09 e Å^{-3}

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

*Cg*1 is the centroid of the C2–C7 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.88 (2)	2.08 (2)	2.955 (2)	174.9 (19)
C4—H4···N2^{ii}	0.93 (3)	2.78 (3)	3.417 (3)	126.99 (18)
C11—H11···N2^{iii}	0.97 (2)	2.70 (2)	3.623 (2)	158.83 (19)
C14—H14*A*···*Cg*1^{iv}	1.02 (2)	2.98 (2)	3.780 (3)	136.3 (2)

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

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).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDSII diffractometer (purchased under grant F.279 of the University Research Fund).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2338).

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[1] 3-Substituted phthalides. Part XXVIII.

  doi:10.1107/S1600536807049677

supplementary materials

Acta Cryst. (2007). E**63**, o4348 [**doi:10.1107/S1600536807049677**]

3-(6-Methyl-2-pyridylamino)isobenzofuran-1(3*H*)-one

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Comment

Phthalides (isobenzofuranones) possess several important properties, such as fungicidal (Aoki *et al.*, 1973; Lacova, 1973), bactericidal and herbicidal (Lacova, 1973), analgesic (Elderfield, 1951), hypertensive and vasorelaxant activities (Tsi & Tan, 1997). In addition, phthalide derivatives are useful in the treatment of circulatory and heart-related diseases (Bellasio, 1974). They are also found to be associated with pesticidal activities (Roy & Sarkar, 2005). Considering the potential interest of such phthalide-3-phosphonates in synthetic organic chemistry, and as agrochemical and pharmaceutical agents, we decided to investigate the solid-state structures of 3-substituted phthalides by X-ray diffraction methods. As part of a continuing study of the interplay between molecular conformation and supramolecular aggregation in 3-substituted phthalides, we report herein the structure of the title compound, (I).

The geometry of the title molecule, (I), (Fig. 1) does not show any significant difference from the average geometry found for 3-anilinoisobenzofuran-1(3*H*) -ones (Büyükgüngör & Odabaşoğlu, 2006*a*,b, 2007; Odabaşoğlu & Büyükgüngör, 2006*a*,b, 2007*a*,b,c). The phthalide group (C1—C8/O2) is planar, the largest deviation from the mean plane being −0.017 (2) Å (for C2). The dihedral angle between the planar phthalide group and phenyl ring is 83.21 (9)°.

In (I), the crystal packing is stabilized by intermolecular N—H···O and C—H···N hydrogen bonds (Table 1, Fig. 2), which generate edge-fused $R_2^1(6)R_4^4(24)R_2^1(6)$ ring motifs (Etter, 1990). These motifs also generate a three dimensional network by C—H···π and π···π interactions (Table 1, Fig. 3), where the π···π interactions occur between (C2—C7) and (C9—C14) rings and their symmetry-related counterparts [symmetry code: x, $1/2 - y$, $1/2 + z$], with a centroid-to-centroid distance of 3.822 (1) Å and a plane to plane separation of 3.697 Å.

Experimental

The title compound was prepared according to the method described by Odabaşoğlu & Büyükgüngör (2006*a*), using phthalaldehydic acid and 2-hydroxy-5-chloroaniline as starting materials (yield; 80%; m.p. 420–422 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution (95%) at room temperature.

Refinement

H atoms were located in a difference syntheses and refined isotropically [N—H = 0.88 (2) Å, U_{iso}(H) = 0.101 (7) Å^2 and C—H = 0.93 (3)–1.02 (2) Å, U_{iso}(H) = 0.075 (5)–0.149 (10) Å^2].

Figures

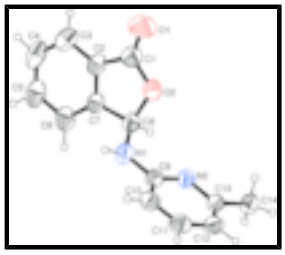

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level

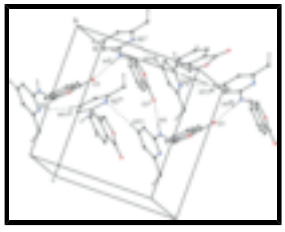

Fig. 2. A partial packing diagram of (I), showing the formation of $R_4^4(24)$ motif [symmetry codes: (i) $x-1, y, z$; (ii) $x-1/2, y, 1/2-z$; (iii) $x-1/2, 1/2-y, 1-z$].

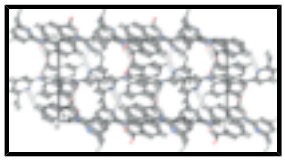

Fig. 3. A partial packing diagram of (I), showing the C—H···N and N—H···O hydrogen bonds along y-axis [symmetry codes: (i) $x-1/2, y, 1/2-z$; (ii) $x-1/2, y-1/2, 1-z$; (iii) $x+1/2, y, 1/2-z$; (iv) $x-1/2, y-1/2, 1-z$].

3-(6-Methyl-2-pyridylamino)isobenzofuran-1(3*H*)-one

Crystal data

$C_{14}H_{12}N_2O_2$	F_{000} = 1008
M_r = 240.26	D_x = 1.292 Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 11933 reflections
a = 10.1367 (7) Å	θ = 1.8–27.2°
b = 22.519 (2) Å	μ = 0.09 mm^{-1}
c = 10.8253 (8) Å	T = 296 K
V = 2471.0 (3) Å^3	Prism, colorless
Z = 8	0.64 × 0.36 × 0.14 mm

Data collection

Stoe IPDSII diffractometer	2437 independent reflections
Radiation source: fine-focus sealed tube	1265 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.056
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 26.0°
T = 296 K	θ_{min} = 1.8°
ω scans	h = −12→12
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	k = −27→27

T_{min} = 0.970, T_{max} = 0.990
17021 measured reflections

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.095$

$S = 0.89$

2437 reflections

212 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.09$ e Å^{-3}

$\Delta\rho_{min} = -0.09$ e Å^{-3}

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

Extinction coefficient: 0.0065 (8)

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	1.04032 (18)	0.07038 (8)	0.25289 (16)	0.1286 (6)
O2	0.90927 (13)	0.10288 (5)	0.40304 (13)	0.0841 (4)
N1	0.68545 (16)	0.10890 (7)	0.46993 (17)	0.0761 (4)
N2	0.75182 (13)	0.18310 (6)	0.60452 (13)	0.0676 (4)
C1	0.9574 (2)	0.06011 (9)	0.3292 (2)	0.0861 (6)
C2	0.89111 (19)	0.00431 (7)	0.35851 (16)	0.0757 (5)
C3	0.9070 (3)	−0.05216 (11)	0.3075 (2)	0.0988 (7)
C4	0.8291 (4)	−0.09672 (11)	0.3527 (3)	0.1144 (9)
C5	0.7376 (3)	−0.08594 (11)	0.4421 (3)	0.1152 (9)
C6	0.7198 (3)	−0.03037 (10)	0.4921 (2)	0.0935 (7)
C7	0.79959 (19)	0.01458 (7)	0.44879 (16)	0.0699 (5)
C8	0.80476 (19)	0.07843 (7)	0.48549 (19)	0.0697 (5)
C9	0.66928 (16)	0.16633 (7)	0.51600 (16)	0.0662 (5)
C10	0.56963 (19)	0.20219 (10)	0.4707 (2)	0.0774 (5)

C11	0.5581 (2)	0.25831 (10)	0.5175 (2)	0.0854 (6)
C12	0.6424 (2)	0.27651 (10)	0.6096 (2)	0.0822 (6)
C13	0.73612 (17)	0.23811 (8)	0.65240 (16)	0.0698 (5)
C14	0.8268 (3)	0.25249 (12)	0.7571 (2)	0.0890 (6)
H1	0.642 (2)	0.0998 (9)	0.402 (2)	0.101 (7)*
H3	0.975 (2)	−0.0544 (9)	0.2473 (19)	0.097 (7)*
H4	0.846 (2)	−0.1345 (13)	0.322 (3)	0.149 (10)*
H5	0.681 (2)	−0.1199 (13)	0.470 (2)	0.145 (9)*
H6	0.652 (2)	−0.0223 (10)	0.555 (2)	0.127 (9)*
H8	0.8356 (16)	0.0860 (7)	0.5700 (17)	0.075 (5)*
H10	0.5152 (18)	0.1888 (8)	0.4067 (18)	0.092 (6)*
H11	0.489 (2)	0.2842 (10)	0.4852 (17)	0.104 (7)*
H12	0.6383 (19)	0.3151 (9)	0.6451 (19)	0.104 (7)*
H14A	0.796 (2)	0.2350 (10)	0.839 (2)	0.125 (8)*
H14B	0.838 (2)	0.2951 (12)	0.767 (2)	0.133 (8)*
H14C	0.914 (3)	0.2369 (10)	0.741 (2)	0.131 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1376 (13)	0.1322 (14)	0.1159 (12)	−0.0053 (11)	0.0510 (11)	0.0183 (10)
O2	0.0910 (9)	0.0629 (7)	0.0984 (9)	−0.0112 (7)	0.0080 (8)	0.0032 (7)
N1	0.0799 (11)	0.0667 (9)	0.0816 (11)	0.0010 (8)	−0.0150 (9)	−0.0069 (8)
N2	0.0709 (9)	0.0630 (9)	0.0688 (9)	−0.0049 (7)	−0.0005 (7)	−0.0018 (7)
C1	0.0979 (15)	0.0846 (14)	0.0760 (13)	0.0008 (12)	0.0063 (12)	0.0061 (11)
C2	0.0993 (14)	0.0608 (11)	0.0671 (11)	0.0033 (10)	−0.0075 (10)	0.0013 (9)
C3	0.132 (2)	0.0886 (17)	0.0760 (14)	0.0162 (15)	−0.0067 (15)	−0.0102 (12)
C4	0.173 (3)	0.0621 (15)	0.108 (2)	0.0023 (17)	−0.029 (2)	−0.0098 (14)
C5	0.156 (3)	0.0672 (16)	0.123 (2)	−0.0222 (16)	−0.0116 (19)	0.0085 (15)
C6	0.1133 (18)	0.0702 (14)	0.0970 (16)	−0.0151 (12)	0.0007 (14)	0.0097 (12)
C7	0.0862 (12)	0.0593 (10)	0.0641 (10)	−0.0044 (9)	−0.0073 (10)	0.0030 (9)
C8	0.0821 (12)	0.0608 (10)	0.0662 (12)	−0.0044 (9)	−0.0026 (10)	−0.0005 (9)
C9	0.0693 (11)	0.0625 (11)	0.0669 (11)	−0.0044 (9)	0.0053 (9)	0.0021 (8)
C10	0.0692 (12)	0.0848 (14)	0.0781 (12)	0.0037 (10)	−0.0038 (11)	0.0058 (11)
C11	0.0792 (14)	0.0812 (14)	0.0958 (16)	0.0155 (11)	0.0072 (12)	0.0070 (12)
C12	0.0846 (14)	0.0691 (13)	0.0930 (15)	0.0054 (11)	0.0195 (12)	−0.0039 (11)
C13	0.0717 (11)	0.0647 (11)	0.0730 (11)	−0.0081 (9)	0.0128 (9)	−0.0058 (9)
C14	0.0944 (17)	0.0871 (15)	0.0855 (16)	−0.0145 (14)	0.0044 (13)	−0.0210 (12)

Geometric parameters (Å, °)

C1—O1	1.201 (2)	C8—H8	0.982 (18)
C1—O2	1.343 (2)	C9—N2	1.327 (2)
C1—C2	1.460 (3)	C9—C10	1.383 (2)
C2—C7	1.367 (2)	C9—N1	1.396 (2)
C2—C3	1.396 (3)	C10—C11	1.367 (3)
C3—C4	1.367 (4)	C10—H10	0.94 (2)
C3—H3	0.95 (2)	C11—C12	1.376 (3)
C4—C5	1.363 (4)	C11—H11	0.97 (2)

C4—H4	0.93 (3)	C12—C13	1.365 (3)
C5—C6	1.375 (4)	C12—H12	0.95 (2)
C5—H5	1.00 (3)	C13—N2	1.352 (2)
C6—C7	1.378 (3)	C13—C14	1.495 (3)
C6—H6	0.99 (2)	C14—H14A	1.02 (2)
C7—C8	1.493 (2)	C14—H14B	0.97 (3)
C8—N1	1.401 (2)	C14—H14C	0.97 (2)
C8—O2	1.491 (2)	N1—H1	0.88 (2)
O1—C1—O2	121.7 (2)	N2—C9—C10	123.38 (17)
O1—C1—C2	129.6 (2)	N2—C9—N1	116.60 (16)
O2—C1—C2	108.70 (18)	C10—C9—N1	120.01 (18)
C7—C2—C3	121.0 (2)	C11—C10—C9	118.1 (2)
C7—C2—C1	108.79 (16)	C11—C10—H10	121.5 (12)
C3—C2—C1	130.2 (2)	C9—C10—H10	120.3 (12)
C4—C3—C2	117.4 (3)	C10—C11—C12	119.4 (2)
C4—C3—H3	128.7 (13)	C10—C11—H11	118.7 (12)
C2—C3—H3	113.8 (13)	C12—C11—H11	121.9 (12)
C5—C4—C3	121.1 (3)	C13—C12—C11	119.3 (2)
C5—C4—H4	122.9 (17)	C13—C12—H12	118.2 (12)
C3—C4—H4	115.9 (17)	C11—C12—H12	122.5 (12)
C4—C5—C6	122.1 (3)	N2—C13—C12	122.15 (18)
C4—C5—H5	118.0 (15)	N2—C13—C14	114.63 (18)
C6—C5—H5	120.0 (15)	C12—C13—C14	123.20 (19)
C5—C6—C7	117.2 (3)	C13—C14—H14A	112.6 (13)
C5—C6—H6	122.1 (14)	C13—C14—H14B	111.6 (14)
C7—C6—H6	120.7 (14)	H14A—C14—H14B	108.8 (19)
C2—C7—C6	121.15 (19)	C13—C14—H14C	110.4 (14)
C2—C7—C8	109.23 (16)	H14A—C14—H14C	107 (2)
C6—C7—C8	129.63 (19)	H14B—C14—H14C	106 (2)
N1—C8—O2	111.15 (15)	C9—N1—C8	120.81 (16)
N1—C8—C7	114.17 (16)	C9—N1—H1	117.0 (13)
O2—C8—C7	102.79 (14)	C8—N1—H1	114.8 (13)
N1—C8—H8	107.6 (10)	C9—N2—C13	117.60 (15)
O2—C8—H8	105.5 (10)	C1—O2—C8	110.47 (14)
C7—C8—H8	115.2 (9)		
O1—C1—C2—C7	−177.3 (2)	N2—C9—C10—C11	1.8 (3)
O2—C1—C2—C7	1.7 (2)	N1—C9—C10—C11	−179.36 (17)
O1—C1—C2—C3	1.0 (4)	C9—C10—C11—C12	−1.9 (3)
O2—C1—C2—C3	−179.99 (19)	C10—C11—C12—C13	0.1 (3)
C7—C2—C3—C4	−1.0 (3)	C11—C12—C13—N2	2.1 (3)
C1—C2—C3—C4	−179.2 (2)	C11—C12—C13—C14	−176.25 (19)
C2—C3—C4—C5	1.5 (4)	N2—C9—N1—C8	−20.1 (2)
C3—C4—C5—C6	−0.7 (4)	C10—C9—N1—C8	160.99 (17)
C4—C5—C6—C7	−0.6 (4)	O2—C8—N1—C9	−73.3 (2)
C3—C2—C7—C6	−0.2 (3)	C7—C8—N1—C9	170.95 (16)
C1—C2—C7—C6	178.32 (18)	C10—C9—N2—C13	0.3 (2)
C3—C2—C7—C8	179.97 (18)	N1—C9—N2—C13	−178.60 (15)
C1—C2—C7—C8	−1.5 (2)	C12—C13—N2—C9	−2.3 (2)

C5—C6—C7—C2	1.0 (3)	C14—C13—N2—C9	176.23 (16)
C5—C6—C7—C8	−179.2 (2)	O1—C1—O2—C8	177.9 (2)
C2—C7—C8—N1	121.33 (18)	C2—C1—O2—C8	−1.1 (2)
C6—C7—C8—N1	−58.5 (3)	N1—C8—O2—C1	−122.34 (17)
C2—C7—C8—O2	0.84 (19)	C7—C8—O2—C1	0.2 (2)
C6—C7—C8—O2	−178.99 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88 (2)	2.08 (2)	2.955 (2)	174.9 (19)
C4—H4···N2^{ii}	0.93 (3)	2.78 (3)	3.417 (3)	126.99 (18)
C11—H11···N2^{iii}	0.97 (2)	2.70 (2)	3.623 (2)	158.83 (19)
C14—H14A···Cg1^{iv}	1.02 (2)	2.98 (2)	3.780 (3)	136.3 (2)

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

Fig. 1

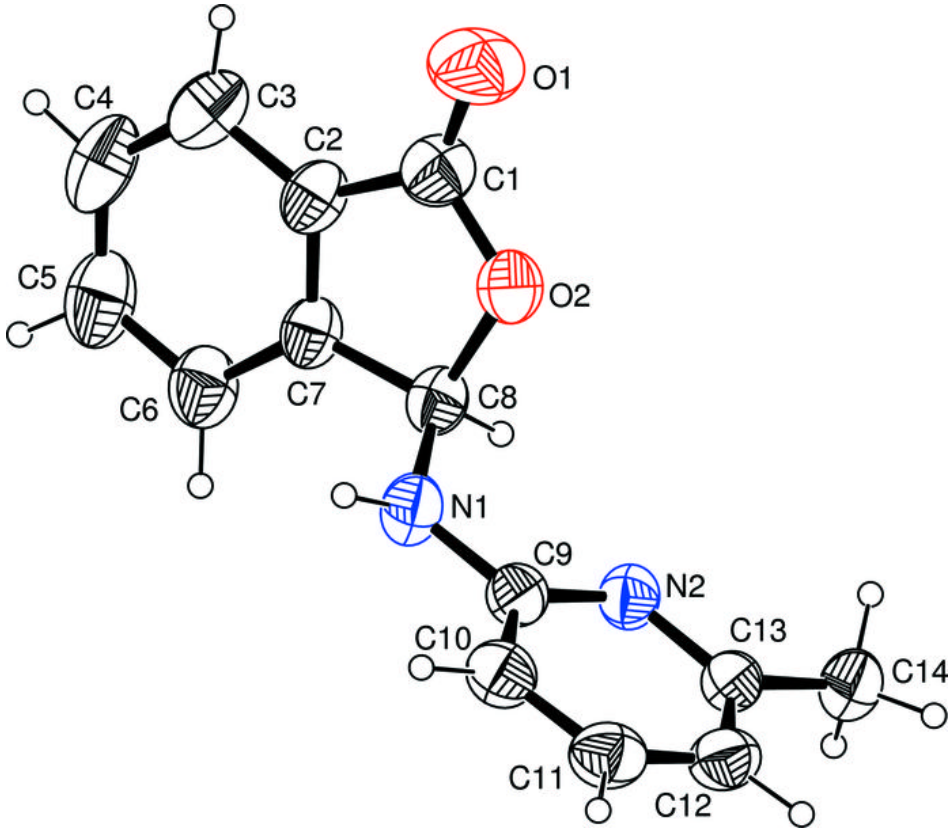

Fig. 2

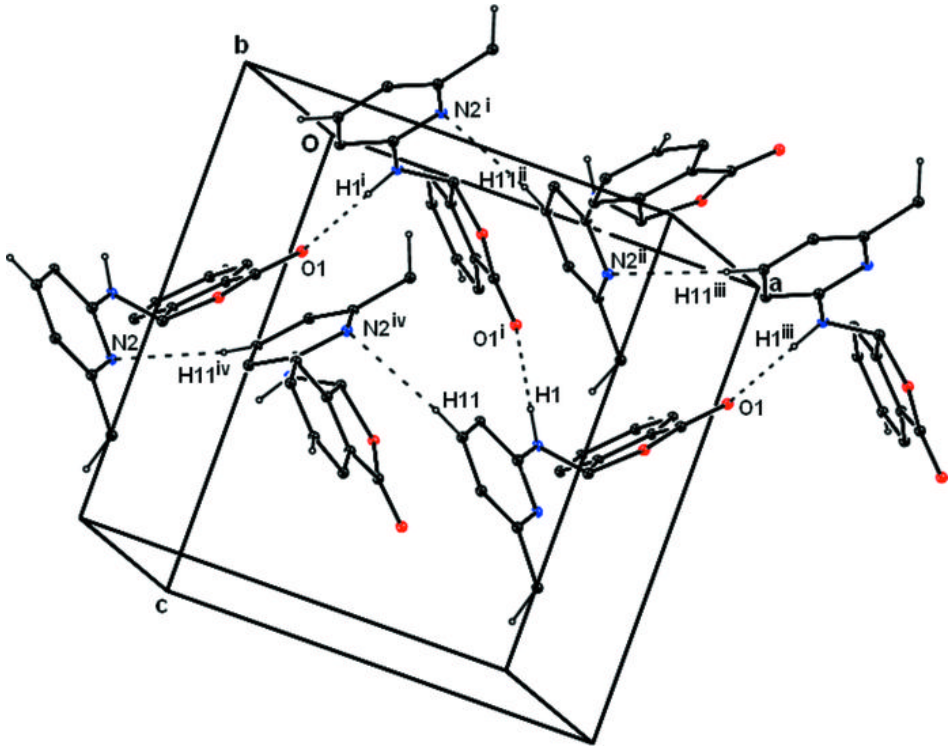
b
O
N2 i
H1i
H11ii
O1
N2ii
H11iii
a
N2
N2iv
O1i
H1iii
H11iv
H11
H1
O1
c

Fig. 3