Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(2-Ethoxyphenyl)-1*H*-benzimidazole monohydrate

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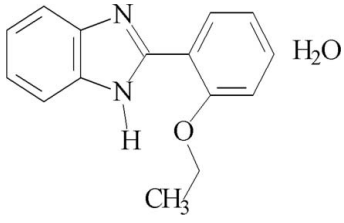
Received 21 September 2007; accepted 27 September 2007

Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.093; data-to-parameter ratio = 10.2.

In the title compound, $C_{15}H_{14}N_2O\cdot H_2O$, the dihedral angle between the benzimidazole ring system and the benzene ring is 6.74 (18)°. The water molecule takes part in the hydrogen-bonding network (N···H—O—H···N), connecting neighboring benzimidazole molecules. The packing is further stabilized by a π–π interaction between two adjacent benzimidazole ring systems, with a distance between the centroids of the benzene rings of 3.8315 (12) Å.

Related literature

For related literature, see: Andrzejewska *et al.* (2002); Bernstein *et al.* (1995); Desiraju (1991); Estrada-Soto *et al.* (2006); Hunter (1994); Küçükbay *et al.* (2003); Lehn (1990); Navarrete-Vázquez *et al.* (2003, 2006); Özden *et al.* (2005).



Experimental

Crystal data

$C_{15}H_{14}N_2O\cdot H_2O$
M_r = 256.30
Monoclinic, $P2_1/c$
a = 7.9148 (16) Å
b = 12.307 (3) Å
c = 13.737 (3) Å
β = 105.49 (3)°
V = 1289.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 297 K
0.27 × 0.23 × 0.19 mm

Data collection

Bruker SMART APEX 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.97, T_{max} = 0.98
7949 measured reflections
2404 independent reflections
2243 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.093
S = 1.09
2404 reflections
236 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.876 (16)	2.153 (16)	2.6848 (16)	118.6 (13)
N1—H1···O2^{i}	0.876 (16)	2.259 (16)	2.9108 (17)	131.1 (14)
O2—H2A···N2^{ii}	0.91 (2)	2.02 (2)	2.9267 (16)	173 (2)
O2—H2B···N2	0.91 (2)	2.02 (2)	2.9170 (17)	171.2 (16)
C13—H13···N2	0.972 (16)	2.486 (15)	2.8427 (19)	101.4 (10)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-NT* (Bruker, 2000); software used to prepare material for publication: *SHELXTL-NT* and *PLATON* (Spek, 2003).

This work was supported by the Consejo Nacional de Ciencia y Tecnología (CONACyT) under grant No. 3562P-E and PROMEP-SEP (GNV).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2213).

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  doi:10.1107/S1600536807047496

supplementary materials

Acta Cryst. (2007). E**63**, o4208 [**doi:10.1107/S1600536807047496**]

2-(2-Ethoxyphenyl)-1*H*-benzimidazole monohydrate

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Comment

Hydrogen bonding and π-π interactions are two of the principal forces which determine structure, self-assembly and recognition in some chemical and biological systems (Lehn, 1990). Benzimidazole and its derivatives are important heterocyclic compounds with versatile pharmacological activities. They have been used as antiparasitic (Navarrete-Vázquez *et al.*, 2003), vasorelaxant and spasmolytic agents (Navarrete-Vázquez *et al.*, 2006; Estrada-Soto *et al.,* 2006), antimicrobial (Özden *et al.*, 2005), antitumoral (Andrzejewska *et al.*, 2002) and antifungal agents (Küçükbay *et al.*, 2003). In our ongoing studies of benzimidazole derivatives as vasorelaxant agents, the compound (I) was prepared by reaction of 1,2-phenylendiamine, with 2-ethoxybenzaldehyde under microwave irradiation.

The whole molecule is non planar; the dihedral angle between benzimidazole moiety and the aryl group is 6.74 (18)° (Fig. 1). The packing can be expressed as a stacking of sheets running along *a* axis. The sheets consist of a two-dimensional hydrogen bonding network (Fig. 2), which is described by the graph set $R^2_4(8)$ (Bernstein *et al.*, 1995). The packing is further stabilized by an offset π-π interaction between two adjacent imidazole molecules, with a distance between the centroids of the C1—C6 and C8—C13 benzene rings (*Cg1* and *Cg2*) of 3.8315 (12) Å (Hunter, 1994; Desiraju, 1991).

Experimental

A mixture of 1,2.phenylendiamine (1.0 g, 9.2 mmol), *2*-ethoxybenzaldehyde (1.52 g, 10 mmol), and sodium metabisulfite (1.92 g, 10 mmol) was stirred and introduced in an open Erlenmeyer Pyrex flask. The mixture was irradiated in a household microwave oven (1000 W) for 40–50 s. After irradiation the mixture was poured onto cold water. The precipitate was collected by filtration, washed with water and dried to give a white solid (m.p. 149.4–150.3 °C). Single crystals of (I) were obtained from a methanol-water (9:1 *v*/*v*) solution (yield 1.93 g, 88%).

Refinement

H atoms were located in a difference Fourier map and were freely refined. Refined C—H, N—H and O—H distances are 0.963 (16)–0.996 (15), 0.879 (16) and 0.91 (2) Å, respectively.

Figures

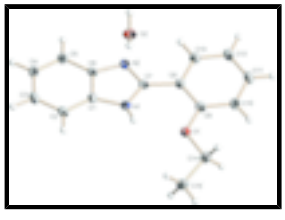

Fig. 1. Perspective view of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

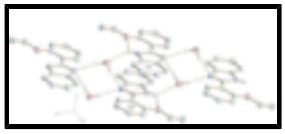

Fig. 2. Crystal packing of (I). The molecules are linked into chains along the *a* axis by intermolecular N···H—O—H···N hydrogen bonds.

2-(2-Ethoxyphenyl)-1*H*-benzimidazole monohydrate

Crystal data

$C_{15}H_{14}N_2O\cdot H_2O$	F_{000} = 544
M_r = 256.30	D_x = 1.320 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 202 reflections
a = 7.9148 (16) Å	θ = 3.6–27.8º
b = 12.307 (3) Å	μ = 0.09 mm^{-1}
c = 13.737 (3) Å	T = 297 K
β = 105.49 (3)º	Plate, colourless
V = 1289.5 (5) Å^3	0.27 × 0.23 × 0.19 mm
Z = 4	

Data collection

Bruker SMART APEX 1000 CCD area-detector diffractometer	2404 independent reflections
Radiation source: fine-focus sealed tube	2243 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
Detector resolution: 8.3 pixels mm^{-1}	θ_{max} = 25.5º
T = 293(2) K	θ_{min} = 2.3º
φ and ω scans	h = −9→9
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	k = −11→14
T_{min} = 0.97, T_{max} = 0.98	l = −16→16
7949 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.037	All H-atom parameters refined
$wR(F^2)$ = 0.093	$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 0.4998P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.09	$(\Delta/\sigma)_{max} < 0.001$
2404 reflections	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
236 parameters	$\Delta\rho_{min}$ = −0.25 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}
C1	−0.05937 (16)	0.47716 (10)	0.84284 (9)	0.0162 (3)
C2	−0.19320 (17)	0.53173 (11)	0.77306 (10)	0.0193 (3)
C3	−0.14220 (18)	0.61769 (12)	0.72245 (10)	0.0218 (3)
C4	0.03411 (18)	0.64841 (11)	0.74050 (10)	0.0218 (3)
C5	0.16608 (18)	0.59365 (11)	0.80924 (10)	0.0202 (3)
C6	0.11740 (16)	0.50595 (10)	0.86018 (9)	0.0164 (3)
C7	0.11019 (16)	0.36787 (10)	0.95614 (9)	0.0155 (3)
C8	0.16812 (16)	0.28158 (10)	1.03137 (9)	0.0167 (3)
C9	0.05569 (16)	0.20205 (11)	1.05285 (9)	0.0176 (3)
C10	0.12096 (18)	0.12488 (11)	1.12797 (10)	0.0209 (3)
C11	0.29693 (18)	0.12576 (11)	1.18019 (10)	0.0223 (3)
C12	0.41012 (18)	0.20236 (11)	1.15903 (10)	0.0221 (3)
C13	0.34549 (17)	0.27953 (11)	1.08530 (10)	0.0199 (3)
C14	−0.23200 (18)	0.12119 (12)	1.01266 (11)	0.0232 (3)
C15	−0.40148 (19)	0.13433 (13)	0.93175 (12)	0.0267 (3)
H1	−0.152 (2)	0.3559 (13)	0.9145 (11)	0.022 (4)*
H2	−0.316 (2)	0.5117 (12)	0.7609 (11)	0.021 (4)*
H3	−0.232 (2)	0.6590 (13)	0.6738 (12)	0.022 (4)*
H4	0.0671 (19)	0.7099 (13)	0.7035 (11)	0.022 (4)*
H5	0.289 (2)	0.6147 (12)	0.8229 (11)	0.020 (4)*
H10	0.044 (2)	0.0704 (13)	1.1430 (11)	0.022 (4)*
H11	0.339 (2)	0.0721 (13)	1.2320 (12)	0.024 (4)*
H12	0.537 (2)	0.2018 (12)	1.1952 (11)	0.022 (4)*
H13	0.4237 (19)	0.3340 (13)	1.0702 (11)	0.019 (4)*
H2A	0.633 (3)	0.4683 (18)	0.9586 (17)	0.055 (6)*
H14A	−0.250 (2)	0.1309 (13)	1.0802 (13)	0.027 (4)*
H15A	−0.455 (2)	0.2055 (16)	0.9349 (13)	0.040 (5)*
H2B	0.466 (3)	0.4167 (15)	0.9152 (13)	0.039 (5)*
H14B	−0.175 (2)	0.0486 (14)	1.0086 (12)	0.025 (4)*
H15B	−0.383 (2)	0.1216 (14)	0.8638 (14)	0.036 (5)*
H15C	−0.486 (2)	0.0807 (15)	0.9417 (13)	0.039 (5)*
N1	−0.05962 (14)	0.38927 (9)	0.90544 (8)	0.0158 (2)
N2	0.22124 (14)	0.43630 (9)	0.93077 (8)	0.0170 (2)

O1	−0.11533 (11)	0.20526 (8)	0.99718 (7)	0.0200 (2)
O2	0.57838 (13)	0.41862 (8)	0.91144 (7)	0.0239 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0194 (6)	0.0158 (7)	0.0140 (6)	0.0008 (5)	0.0057 (5)	−0.0023 (5)
C2	0.0169 (7)	0.0224 (7)	0.0174 (6)	0.0021 (5)	0.0027 (5)	−0.0010 (5)
C3	0.0244 (7)	0.0220 (7)	0.0174 (6)	0.0052 (6)	0.0028 (5)	0.0020 (5)
C4	0.0280 (7)	0.0189 (7)	0.0191 (7)	−0.0002 (6)	0.0073 (5)	0.0029 (6)
C5	0.0199 (7)	0.0208 (7)	0.0204 (7)	−0.0019 (5)	0.0061 (5)	−0.0006 (5)
C6	0.0174 (6)	0.0176 (7)	0.0137 (6)	0.0010 (5)	0.0032 (5)	−0.0026 (5)
C7	0.0162 (6)	0.0160 (7)	0.0142 (6)	−0.0002 (5)	0.0040 (5)	−0.0033 (5)
C8	0.0188 (6)	0.0173 (7)	0.0144 (6)	0.0016 (5)	0.0052 (5)	−0.0018 (5)
C9	0.0180 (6)	0.0191 (7)	0.0158 (6)	0.0011 (5)	0.0047 (5)	−0.0023 (5)
C10	0.0243 (7)	0.0193 (7)	0.0197 (7)	−0.0012 (6)	0.0069 (5)	0.0017 (5)
C11	0.0257 (7)	0.0216 (7)	0.0183 (7)	0.0049 (6)	0.0040 (5)	0.0037 (6)
C12	0.0191 (7)	0.0251 (8)	0.0204 (7)	0.0030 (6)	0.0023 (5)	0.0006 (6)
C13	0.0192 (7)	0.0201 (7)	0.0203 (7)	−0.0007 (5)	0.0051 (5)	−0.0002 (5)
C14	0.0220 (7)	0.0217 (8)	0.0264 (8)	−0.0046 (6)	0.0069 (6)	0.0037 (6)
C15	0.0210 (7)	0.0244 (8)	0.0325 (8)	−0.0061 (6)	0.0033 (6)	0.0012 (6)
N1	0.0138 (5)	0.0172 (6)	0.0167 (5)	−0.0010 (4)	0.0045 (4)	−0.0003 (4)
N2	0.0168 (5)	0.0176 (6)	0.0161 (5)	−0.0006 (4)	0.0034 (4)	−0.0002 (4)
O1	0.0169 (5)	0.0208 (5)	0.0206 (5)	−0.0040 (4)	0.0022 (4)	0.0037 (4)
O2	0.0179 (5)	0.0276 (6)	0.0264 (5)	−0.0026 (4)	0.0064 (4)	−0.0067 (4)

Geometric parameters (Å, °)

C1—N1	1.3821 (17)	C9—C10	1.3961 (19)
C1—C2	1.3962 (18)	C10—C11	1.386 (2)
C1—C6	1.4006 (18)	C10—H10	0.965 (16)
C2—C3	1.384 (2)	C11—C12	1.384 (2)
C2—H2	0.969 (15)	C11—H11	0.963 (16)
C3—C4	1.402 (2)	C12—C13	1.3831 (19)
C3—H3	0.977 (16)	C12—H12	0.996 (15)
C4—C5	1.382 (2)	C13—H13	0.972 (16)
C4—H4	0.985 (16)	C14—O1	1.4399 (16)
C5—C6	1.3955 (19)	C14—C15	1.505 (2)
C5—H5	0.974 (15)	C14—H14A	0.984 (16)
C6—N2	1.3873 (17)	C14—H14B	1.008 (17)
C7—N2	1.3292 (17)	C15—H15A	0.979 (19)
C7—N1	1.3641 (17)	C15—H15B	0.994 (19)
C7—C8	1.4673 (18)	C15—H15C	0.977 (19)
C8—C13	1.4016 (19)	N1—H1	0.879 (16)
C8—C9	1.4062 (18)	O2—H2A	0.91 (2)
C9—O1	1.3659 (16)	O2—H2B	0.91 (2)
N1—C1—C2	132.58 (12)	C9—C10—H10	120.0 (9)
N1—C1—C6	105.04 (11)	C12—C11—C10	120.94 (13)

C2—C1—C6	122.36 (12)	C12—C11—H11	120.4 (9)
C3—C2—C1	116.30 (12)	C10—C11—H11	118.7 (9)
C3—C2—H2	121.3 (9)	C13—C12—C11	119.21 (13)
C1—C2—H2	122.4 (9)	C13—C12—H12	119.8 (9)
C2—C3—C4	121.81 (13)	C11—C12—H12	121.0 (9)
C2—C3—H3	119.1 (9)	C12—C13—C8	121.45 (13)
C4—C3—H3	119.1 (9)	C12—C13—H13	119.9 (9)
C5—C4—C3	121.61 (13)	C8—C13—H13	118.7 (9)
C5—C4—H4	118.1 (9)	O1—C14—C15	107.10 (11)
C3—C4—H4	120.3 (9)	O1—C14—H14A	108.2 (9)
C4—C5—C6	117.41 (12)	C15—C14—H14A	111.0 (9)
C4—C5—H5	122.3 (9)	O1—C14—H14B	108.5 (9)
C6—C5—H5	120.3 (9)	C15—C14—H14B	112.1 (9)
N2—C6—C5	129.57 (12)	H14A—C14—H14B	109.8 (13)
N2—C6—C1	109.94 (11)	C14—C15—H15A	112.0 (10)
C5—C6—C1	120.49 (12)	C14—C15—H15B	110.6 (10)
N2—C7—N1	111.97 (11)	H15A—C15—H15B	110.9 (15)
N2—C7—C8	122.62 (11)	C14—C15—H15C	109.6 (11)
N1—C7—C8	125.40 (12)	H15A—C15—H15C	105.9 (14)
C13—C8—C9	118.50 (12)	H15B—C15—H15C	107.6 (14)
C13—C8—C7	117.76 (12)	C7—N1—C1	107.69 (11)
C9—C8—C7	123.74 (12)	C7—N1—H1	125.7 (10)
O1—C9—C10	123.32 (12)	C1—N1—H1	126.5 (10)
O1—C9—C8	116.77 (11)	C7—N2—C6	105.36 (10)
C10—C9—C8	119.91 (12)	C9—O1—C14	118.37 (10)
C11—C10—C9	119.97 (13)	H2A—O2—H2B	105.4 (17)
C11—C10—H10	120.0 (9)		
N1—C1—C2—C3	−179.46 (13)	O1—C9—C10—C11	178.94 (12)
C6—C1—C2—C3	−0.97 (19)	C8—C9—C10—C11	−1.0 (2)
C1—C2—C3—C4	−0.2 (2)	C9—C10—C11—C12	0.0 (2)
C2—C3—C4—C5	0.6 (2)	C10—C11—C12—C13	0.6 (2)
C3—C4—C5—C6	0.2 (2)	C11—C12—C13—C8	−0.2 (2)
C4—C5—C6—N2	178.69 (12)	C9—C8—C13—C12	−0.75 (19)
C4—C5—C6—C1	−1.28 (19)	C7—C8—C13—C12	178.61 (12)
N1—C1—C6—N2	0.61 (13)	N2—C7—N1—C1	0.12 (14)
C2—C1—C6—N2	−178.24 (11)	C8—C7—N1—C1	179.17 (11)
N1—C1—C6—C5	−179.41 (11)	C2—C1—N1—C7	178.24 (13)
C2—C1—C6—C5	1.74 (19)	C6—C1—N1—C7	−0.44 (13)
N2—C7—C8—C13	6.74 (18)	N1—C7—N2—C6	0.26 (14)
N1—C7—C8—C13	−172.21 (12)	C8—C7—N2—C6	−178.82 (11)
N2—C7—C8—C9	−173.93 (12)	C5—C6—N2—C7	179.48 (13)
N1—C7—C8—C9	7.1 (2)	C1—C6—N2—C7	−0.54 (14)
C13—C8—C9—O1	−178.58 (11)	C10—C9—O1—C14	−3.68 (18)
C7—C8—C9—O1	2.10 (18)	C8—C9—O1—C14	176.24 (11)
C13—C8—C9—C10	1.34 (18)	C15—C14—O1—C9	−171.40 (11)
C7—C8—C9—C10	−177.98 (12)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.876 (16)	2.153 (16)	2.6848 (16)	118.6 (13)
N1—H1···O2^{i}	0.876 (16)	2.259 (16)	2.9108 (17)	131.1 (14)
O2—H2A···N2^{ii}	0.91 (2)	2.02 (2)	2.9267 (16)	173 (2)
O2—H2B···N2	0.91 (2)	2.02 (2)	2.9170 (17)	171.2 (16)
C13—H13···N2	0.972 (16)	2.486 (15)	2.8427 (19)	101.4 (10)

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

Fig. 1

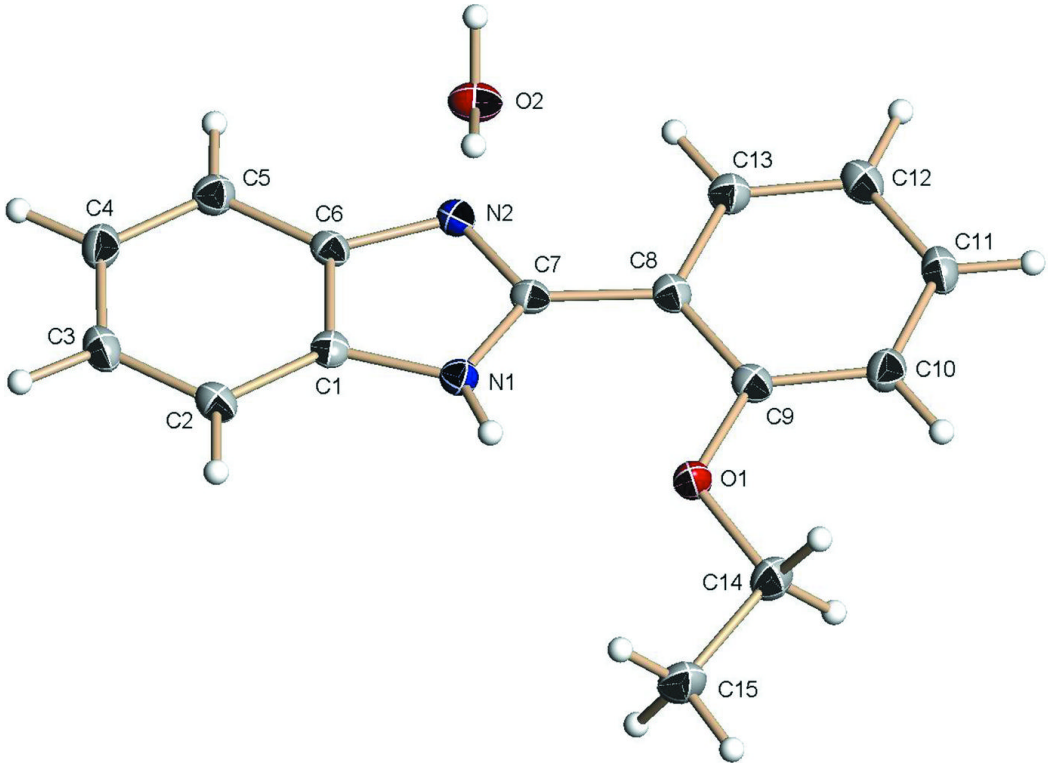

Fig. 2