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4-(1*H*-Benzo[*d*]imidazol-2-yl)phenol

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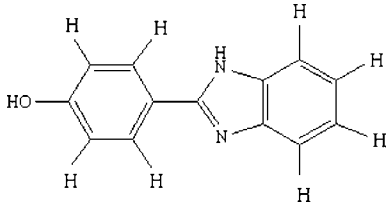
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.103; data-to-parameter ratio = 16.5.

In the title compound, $C_{13}H_{10}N_2O$, the benzimidazole system is nearly coplanar with the phenol ring, with a small dihedral angle of 8.11 (5)°. Intermolecular N—H···O and O—H···N hydrogen bonding helps to stabilize the crystal structure.

Related literature

For general background, see Cai, Chen *et al.* (2003). For related structures, see Cai, Su *et al.* (2003); Su *et al.* (2002). For related literature, see: Cai (2002).



Experimental

Crystal data

$C_{13}H_{10}N_2O$
M_r = 210.23
Monoclinic, $P2_1/n$
a = 7.1679 (3) Å
b = 15.1517 (6) Å
c = 9.9079 (4) Å
β = 90.556 (2)°
V = 1076.01 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.22 × 0.17 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
10089 measured reflections
2464 independent reflections
2092 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.103
S = 1.04
2464 reflections
149 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N2^{i}	0.82	1.84	2.6515 (12)	174
N1—H1···O1^{ii}	0.886 (8)	2.012 (9)	2.8564 (12)	158.8 (12)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2292).

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supplementary materials

Acta Cryst. (2007). E**63**, o3470 [**doi:10.1107/S1600536807033612**]

4-(1*H*-Benzo[*d*]imidazol-2-yl)phenol

Q.-G. Zhan, M.-S. Liu, R.-H. Zeng, D.-Q. Yang and Y.-P. Cai

Comment

The ligands containing benzimidazolyl substituent(*s*), which could provide hydrogen bond donor NH groups and π-π stacking interaction, have being extensively investigated now (Cai, Chen *et al.*, 2003). As a part of the structural studies of benzimidazolyl series (Cai *et al.*, 2002; Cai, Su *et al.* 2003) here we report the synthesis and structure of the title compound.

Fig. 1 shows an *ORTEP* diagram of the compound together with the atom numbering scheme. The benzimidazolyl ring is almost coplanar to phenol ring with 8.11 (1)° of dihedral angle in the molecule. The dihedral angle between two perpendicular sheet-like molecules is 86.19 (6)° in the crystal structure, which are connected by hydrogen bondings N—H···O [O···N 2.856 (1) Å, H···O 2.012 (2) Å, N—H···O 158.8 (1)° [symmetry code: $x - 1/2,-y + 1/2,z + 1/2$] and O—H···N [O···N 2.652 (1) Å, H···O 1.843 (1) Å, O—H···N 173.5 (2)° [symmetry code: $x - 1/2,-y + 1/2,z - 1/2$] to form an infinite wave-like two-dimensional layer, while the three-dimensional network structure is constructed by face-to-face π-π stacking interaction, the shortest distance between benzimidazole ring and phenol ring is 3.554 Å.

Experimental

To phenylenediamine (3.67 g, 0.034 mol) in propylene glycol (50 ml) was added 4-hydroxybenzoic acid (4.69 g, 0.034 mol), and the solution refluxed for 24 h and then cooled to room temperature. Ice cold water (50 ml) was then added to force the precipitation of a brown solid which was collected and dissolved in hot methanol. The solution is filtered over activated carbon and the filtrate was allowed to evaporate slowly to give single crystals (yield 6.15 g, 86%).

Refinement

H atoms on C and O atoms were placed in idealized positions, and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(O). H atom on N atom was located in a difference Fourier map and refined isotropically.

Figures

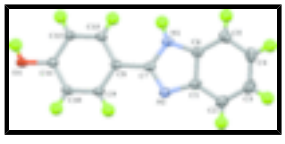

Fig. 1. The structure of title molecule. The atom-numbering scheme is shown at the 30% probability level.

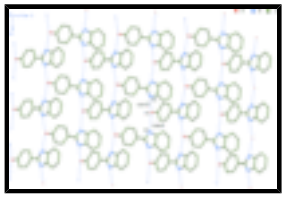

Fig. 2. A view of the molecular network parallel to (101)

4-(1*H*-Benzo[*d*]imidazol-2-yl)phenol

Crystal data

$C_{13}H_{10}N_2O$	$F_{000} = 440$
$M_r = 210.23$	$D_x = 1.298$ Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 508 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.1679$ (3) Å	Cell parameters from 5172 reflections
$b = 15.1517$ (6) Å	$\theta = 2.4$–27.5º
$c = 9.9079$ (4) Å	$\mu = 0.09$ mm^{-1}
$\beta = 90.556$ (2)º	$T = 298$ (2) K
$V = 1076.01$ (8) Å^3	Block, colourless
$Z = 4$	0.22 × 0.17 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2092 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.019$
Monochromator: graphite	$\theta_{max} = 27.5$º
$T = 298$(2) K	$\theta_{min} = 2.4$º
φ and ω scans	$h = -9 \rightarrow 9$
Absorption correction: none	$k = -19 \rightarrow 15$
10089 measured reflections	$l = -12 \rightarrow 12$
2464 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.103$	$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 0.1927P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
2464 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
149 parameters	$\Delta\rho_{min} = -0.17$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. The assigned structure was substantiated by EA and MS data. Elemental analysis calculated for $C_{13}H_{10}N_2O$: C, 74.27; H, 4.79; N, 13.33; found: C, 73.98; H, 4.87; N, 13.28. FAB-MS m/*z* (%): 211(M^++1, 68), 210(M^+, 100).

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	0.12380 (10)	0.35627 (6)	0.15835 (9)	0.0498 (2)
H1A	0.0185	0.3760	0.1462	0.075*
N2	0.29490 (13)	0.06719 (6)	0.61996 (10)	0.0455 (2)
N1	−0.01358 (12)	0.06759 (6)	0.63364 (10)	0.0406 (2)
C1	0.24064 (16)	0.00742 (8)	0.71879 (12)	0.0460 (3)
C2	0.3466 (2)	−0.04686 (10)	0.80335 (16)	0.0646 (4)
H2	0.4761	−0.0477	0.7984	0.078*
C3	0.2541 (2)	−0.09910 (10)	0.89419 (16)	0.0691 (4)
H3	0.3225	−0.1360	0.9511	0.083*
C4	0.0615 (2)	−0.09817 (9)	0.90314 (14)	0.0614 (4)
H4	0.0036	−0.1344	0.9659	0.074*
C5	−0.04601 (19)	−0.04497 (9)	0.82150 (13)	0.0522 (3)
H5	−0.1754	−0.0442	0.8278	0.063*
C6	0.04717 (15)	0.00766 (7)	0.72905 (11)	0.0412 (3)
C7	0.13874 (14)	0.10192 (7)	0.57169 (11)	0.0381 (2)
C8	0.12968 (14)	0.16878 (7)	0.46561 (10)	0.0381 (2)
C9	0.29061 (15)	0.19137 (8)	0.39541 (12)	0.0448 (3)
H9	0.4029	0.1639	0.4175	0.054*
C10	0.28632 (15)	0.25331 (8)	0.29430 (12)	0.0467 (3)
H10	0.3953	0.2671	0.2487	0.056*
C11	0.12059 (15)	0.29563 (8)	0.25943 (11)	0.0407 (3)
C12	−0.04087 (15)	0.27377 (8)	0.32846 (12)	0.0446 (3)
H12	−0.1528	0.3016	0.3065	0.054*
C13	−0.03603 (15)	0.21105 (8)	0.42931 (11)	0.0435 (3)
H13	−0.1455	0.1967	0.4739	0.052*
H1	−0.1306 (13)	0.0848 (9)	0.6208 (13)	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

O1	0.0285 (4)	0.0655 (6)	0.0555 (5)	0.0017 (4)	0.0022 (3)	0.0137 (4)
N2	0.0315 (5)	0.0487 (5)	0.0563 (6)	0.0007 (4)	−0.0027 (4)	0.0007 (4)
N1	0.0295 (5)	0.0450 (5)	0.0473 (5)	0.0007 (4)	−0.0001 (4)	−0.0024 (4)
C1	0.0390 (6)	0.0444 (6)	0.0546 (7)	0.0011 (5)	−0.0036 (5)	−0.0013 (5)
C2	0.0470 (7)	0.0663 (9)	0.0804 (10)	0.0077 (6)	−0.0102 (7)	0.0127 (7)
C3	0.0730 (10)	0.0614 (9)	0.0727 (9)	0.0062 (7)	−0.0139 (8)	0.0164 (7)
C4	0.0737 (9)	0.0539 (8)	0.0567 (7)	−0.0047 (7)	0.0002 (7)	0.0068 (6)
C5	0.0504 (7)	0.0523 (7)	0.0540 (7)	−0.0044 (5)	0.0037 (5)	−0.0011 (6)
C6	0.0399 (6)	0.0391 (5)	0.0445 (6)	0.0003 (4)	−0.0018 (4)	−0.0066 (4)
C7	0.0302 (5)	0.0402 (6)	0.0438 (5)	−0.0007 (4)	−0.0012 (4)	−0.0090 (4)
C8	0.0320 (5)	0.0418 (6)	0.0405 (5)	−0.0017 (4)	−0.0009 (4)	−0.0065 (4)
C9	0.0281 (5)	0.0536 (7)	0.0525 (6)	0.0035 (4)	−0.0005 (4)	−0.0002 (5)
C10	0.0272 (5)	0.0599 (7)	0.0532 (6)	−0.0010 (5)	0.0049 (4)	0.0041 (5)
C11	0.0309 (5)	0.0489 (6)	0.0422 (6)	−0.0023 (4)	−0.0010 (4)	−0.0020 (5)
C12	0.0269 (5)	0.0573 (7)	0.0497 (6)	0.0031 (5)	0.0001 (4)	0.0025 (5)
C13	0.0284 (5)	0.0554 (7)	0.0467 (6)	−0.0011 (4)	0.0036 (4)	−0.0002 (5)

Geometric parameters (Å, °)

O1—C11	1.3595 (14)	C4—H4	0.9300
O1—H1A	0.8200	C5—C6	1.3902 (17)
N2—C7	1.3221 (14)	C5—H5	0.9300
N2—C1	1.3920 (15)	C7—C8	1.4609 (16)
N1—C7	1.3610 (14)	C8—C13	1.3935 (15)
N1—C6	1.3784 (15)	C8—C9	1.3953 (15)
N1—H1	0.886 (8)	C9—C10	1.3728 (17)
C1—C6	1.3915 (16)	C9—H9	0.9300
C1—C2	1.3939 (18)	C10—C11	1.3906 (15)
C2—C3	1.374 (2)	C10—H10	0.9300
C2—H2	0.9300	C11—C12	1.3901 (15)
C3—C4	1.384 (2)	C12—C13	1.3792 (16)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.3733 (19)	C13—H13	0.9300
C11—O1—H1A	109.5	C5—C6—C1	122.15 (11)
C7—N2—C1	105.79 (9)	N2—C7—N1	111.40 (10)
C7—N1—C6	108.16 (9)	N2—C7—C8	124.60 (10)
C7—N1—H1	125.8 (9)	N1—C7—C8	124.00 (9)
C6—N1—H1	125.8 (9)	C13—C8—C9	117.74 (11)
C6—C1—N2	109.58 (10)	C13—C8—C7	122.42 (10)
C6—C1—C2	119.69 (12)	C9—C8—C7	119.83 (10)
N2—C1—C2	130.72 (12)	C10—C9—C8	121.24 (10)
C3—C2—C1	118.03 (13)	C10—C9—H9	119.4
C3—C2—H2	121.0	C8—C9—H9	119.4
C1—C2—H2	121.0	C9—C10—C11	120.63 (10)
C2—C3—C4	121.61 (13)	C9—C10—H10	119.7
C2—C3—H3	119.2	C11—C10—H10	119.7
C4—C3—H3	119.2	O1—C11—C12	122.93 (10)
C5—C4—C3	121.50 (14)	O1—C11—C10	118.30 (10)
C5—C4—H4	119.2	C12—C11—C10	118.76 (11)

C3—C4—H4	119.2	C13—C12—C11	120.36 (10)
C4—C5—C6	117.02 (13)	C13—C12—H12	119.8
C4—C5—H5	121.5	C11—C12—H12	119.8
C6—C5—H5	121.5	C12—C13—C8	121.27 (10)
N1—C6—C5	132.78 (11)	C12—C13—H13	119.4
N1—C6—C1	105.07 (10)	C8—C13—H13	119.4
C7—N2—C1—C6	−0.36 (13)	C6—N1—C7—N2	0.72 (12)
C7—N2—C1—C2	−179.12 (14)	C6—N1—C7—C8	−179.15 (9)
C6—C1—C2—C3	0.4 (2)	N2—C7—C8—C13	−172.12 (11)
N2—C1—C2—C3	179.05 (13)	N1—C7—C8—C13	7.74 (16)
C1—C2—C3—C4	−0.4 (2)	N2—C7—C8—C9	8.78 (16)
C2—C3—C4—C5	0.0 (2)	N1—C7—C8—C9	−171.36 (10)
C3—C4—C5—C6	0.3 (2)	C13—C8—C9—C10	0.21 (17)
C7—N1—C6—C5	178.88 (12)	C7—C8—C9—C10	179.36 (11)
C7—N1—C6—C1	−0.89 (12)	C8—C9—C10—C11	0.26 (19)
C4—C5—C6—N1	−179.96 (12)	C9—C10—C11—O1	−179.84 (11)
C4—C5—C6—C1	−0.23 (18)	C9—C10—C11—C12	−0.28 (18)
N2—C1—C6—N1	0.77 (13)	O1—C11—C12—C13	179.35 (11)
C2—C1—C6—N1	179.70 (12)	C10—C11—C12—C13	−0.18 (18)
N2—C1—C6—C5	−179.02 (10)	C11—C12—C13—C8	0.67 (18)
C2—C1—C6—C5	−0.10 (18)	C9—C8—C13—C12	−0.68 (17)
C1—N2—C7—N1	−0.22 (12)	C7—C8—C13—C12	−179.80 (10)
C1—N2—C7—C8	179.65 (10)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···N2^{i}	0.82	1.84	2.6515 (12)	174
N1—H1···O1^{ii}	0.886 (8)	2.012 (9)	2.8564 (12)	158.8 (12)

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

Fig. 1

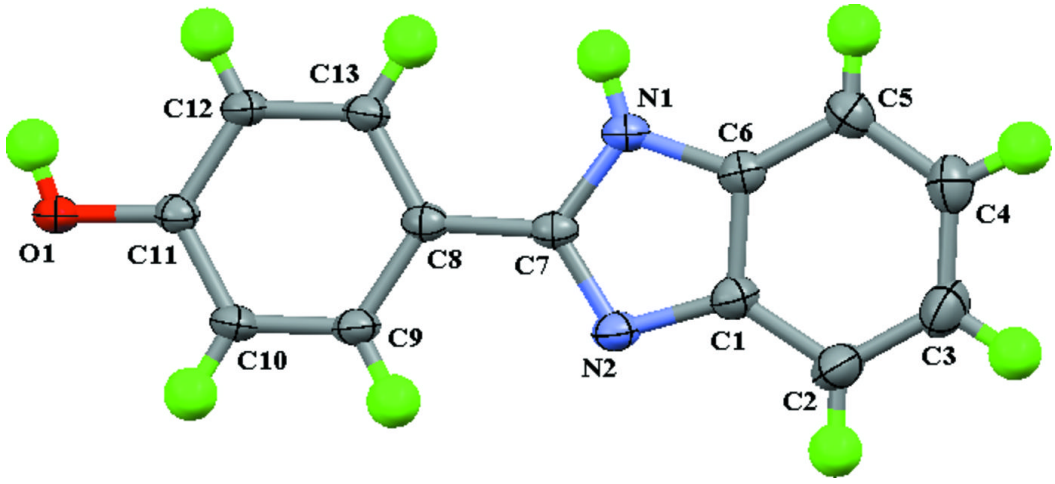

Fig. 2