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2-(2-Hydroxyphenyl)-1,3-benzoxazole

Yi-Ping Tong

Department of Chemistry, Hanshan Normal College, 521041 Chaozhou, People's Republic of China

Correspondence e-mail: typ2469@163.com

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Key indicators

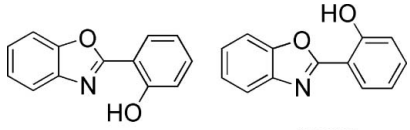
Single-crystal X-ray study
T = 293 K
Mean σ(N–C) = 0.005 Å
Disorder in main residue
R factor = 0.059
wR factor = 0.170
Data-to-parameter ratio = 9.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The molecule of the title compound, $C_{13}H_9NO_2$, is planar, and is disordered so that there are two conformations (1:1) of the phenol ring with respect to the benzoxazole group. Strong intermolecular π–π interactions are noted in the crystal structure.

Comment

There has been growing interest in heterocyclic compounds with O and N heteroatoms, owing to their potential use in electroluminescence. For example, the oxadiazole derivative, 2-biphenyl-4-yl-5-(4-*tert*-butyl-phenyl)-[1,3,4]oxadiazole (PBD), is widely used as an electron-transfer material in electroluminescence devices (Kido & Okamoto, 2002). Similarly, oxazole derivatives are often used as light-emitting materials, such as bis[2-(2-hydroxyphenyl)benzoxazolato]-zinc(II) and -beryllium(II); the former is excellent in terms of electroluminescence (Hamada *et al.*, 1996), while the latter exhibits excellent photoluminescence characteristics (Tong *et al.*, 2005).



(I)

2-(2-Hydroxyphenyl)-1,3-benzoxazole, (I), has been known for decades and is available commercially. Despite this, its crystal structure has not been reported to date. A Be^{II} derivative, $(C_{13}H_8BeNO_2)_2$, has been crystallographically verified (Tong *et al.*, 2005), as has the related 4-methyl-substituted Mn^{III} complex (Asada *et al.*, 1999).

The structure of (I) was determined as a part of programme studying its photoluminescence. The crystallographically determined structure of (I) exhibits disorder owing to a

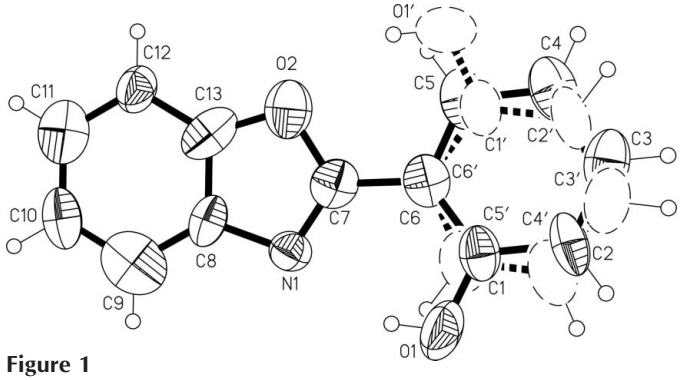


Figure 1
A view of (I), with displacement ellipsoids drawn at the 50% probability level. One of the disordered phenol rings is shown as broken ellipses.

rotation about the bond linking the benzoxazole and phenol rings. From refinement, the conformations were equally present.

In the molecule of (I) (Fig. 1 and Table 1), the geometric parameters are similar to those found in (I) co-crystallized with a Pt^{V} complex (Furuhashi *et al.*, 1991) and those documented for a similar compound, 1-benzooxazol-2-yl-naphthalen-2-ol (Asada *et al.*, 2002), as well as those in its Be^{II} complex (Tong *et al.*, 2005).

Despite the observed disorder, (I) is still planar, as seen in the dihedral angle between the benzoxazole and phenol rings of approximately 3°, as found in the structures mentioned above. This observation is readily related to the strong intramolecular hydrogen bonds, *viz*. O—H···O 2.743 (9) Å and O—H···N 2.686 (8) Å (Table 2); owing to the modelled orientational disorder, each of these intramolecular interactions has 50% contribution.

Strong $\pi-\pi$ stacking interactions, with an interplanar distance of approximately 3.58 Å, link adjacent molecules in a head-to-head style, rendering them into chains, as shown in Fig. 2.

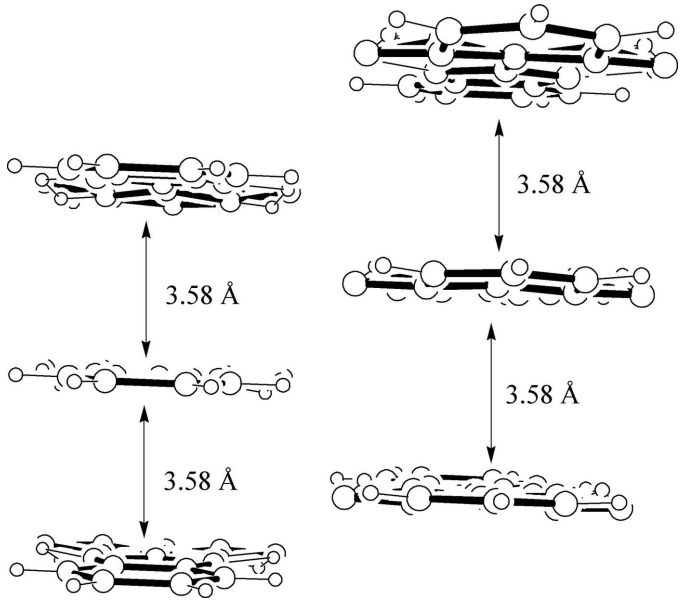


Figure 2
A perspective view of the intermolecular π–π interactions and stacking pattern in (I).

Experimental

2-(2-Hydroxyphenyl)-1,3-benzoxazole, (I), was purchased from Aldrich and crystallized by slow evaporation over several days of an ethanol solution of (I).

Crystal data

$C_{13}H_9NO_2$
M_r = 211.21
Orthorhombic, $Pna2_1$
a = 22.446 (3) Å
b = 3.8547 (5) Å
c = 11.5504 (15) Å
V = 999.4 (2) Å^3
Z = 4
D_x = 1.404 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1095 reflections
θ = 2.5–23.7°
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, colourless
0.40 × 0.23 × 0.18 mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.983
5770 measured reflections
1272 independent reflections
935 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 28.2°
$h = -26 \rightarrow 29$
$k = -5 \rightarrow 4$
$l = -14 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.170
S = 1.08
1272 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.079P)^2 + 0.2556P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Selected geometric parameters (Å).

O1—C1	1.325 (8)	C7—O2	1.383 (6)
C6—C7	1.450 (4)	C8—N1	1.401 (4)
C7—N1	1.269 (6)	C13—O2	1.329 (4)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1′—H1′···O2	0.82	2.00	2.743 (9)	150
O1—H1···N1	0.82	1.97	2.686 (8)	146

In the refinement of (I), the phenol ring has orientational disorder with respect to the benzoxazole group. From refinement, the occupancy factors were found to be equivalent; the refined occupancies were 0.5 (2):0.5 (2). The geometric parameters for each six-membered ring were restrained so that C—C = 1.39 (1) Å. Additionally, the C—O distances were restrained to be equal. The H atoms were placed in calculated positions in the riding-model approximation, with C—H = 0.93 Å and O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O). In the absence of significant anomalous scattering, Friedel pairs were merged.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXL97*.

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