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1-Benzyl-2-[2-(benzyloxy)phenyl]-1*H*-benzimidazole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.110
Data-to-parameter ratio = 8.9

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

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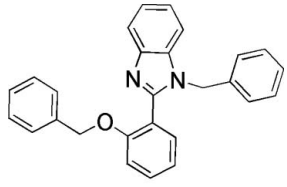
The title compound, $C_{27}H_{22}N_2O$, was prepared by reaction of 2-(2-hydroxyphenyl)benzimidazole with chloromethylbenzene under reflux. The large steric effect of the benzyl substituents results in the phenolate rings and benzimidazole rings being non-coplanar. This is responsible for the observed weak photoluminescence. The crystal structure is determined by intermolecular van der Waals interactions. No hydrogen-bond interactions or π–π stacking interactions were found, which is somewhat unusual for an aromatic heterocyclic compound.

Comment

There is growing interest in benzimidazole and its derivatives for their photoluminescent properties (Tong *et al.*, 2005; Wu *et al.*, 2003; Svejda *et al.*, 1978). 2-(2-Hydroxyphenyl)benzimidazole is an excellent photoluminescent material with an emitting wavelength of 444 nm in the solid state; moreover, its metal complexes with Be^{II} ions have also shown excellent blue-light emitting properties. This is shared by the analogs 2-(2-hydroxyphenyl)benzoxazole and 2-(2-hydroxyphenyl)benzothiazole, as well as their Be^{II} complexes. This is partly due to the fact that these ligands, before and after coordination to Be^{II} ions, are basically coplanar or only slightly distorted, with the dihedral angles between phenolate and benzimidazole rings being less than 10° (Tong *et al.*, 2005).



(I)

Ligand distortion can generate larger dihedral angles between phenolate and benzimidazole moieties, and result in the reduction of light-emitting capacity. For example, 2-(2-ethoxyphenyl)-1-ethyl-1*H*-benzimidazole, exhibits inferior light-emitting properties than its parent compound 2-(2-hydroxyphenyl)benzimidazole, owing to the larger deviation from coplanarity (Tong & Li, 2004). In our attempt to synthesize the *N*,*O*-donor ligand 2-(1-benzyl-1*H*-benzimidazol-2-yl)phenol to obtain a blue-light emitting complex with metal ions, we obtained another weakly photoluminescent compound, the title compound, (I).

In the crystal structure of (I) (Fig. 1), the C—C, C—O and C—N bond lengths are similar to those found in 2-(2-ethoxyphenyl)-1-ethyl-1*H*-benzimidazole (Tong & Li, 2004), its parent compound, 2-(2-hydroxyphenyl)benzimidazole

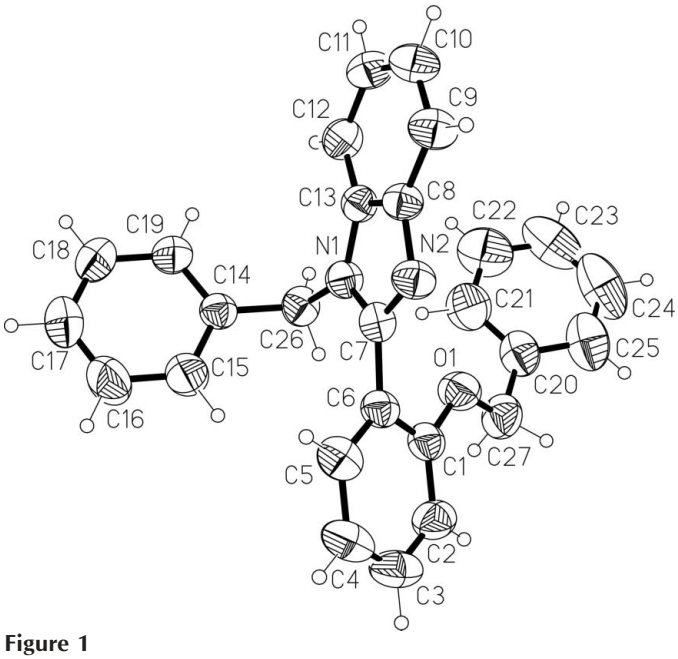


Figure 1
View (*SHELXTL*; Sheldrick, 2000) of the molecules of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

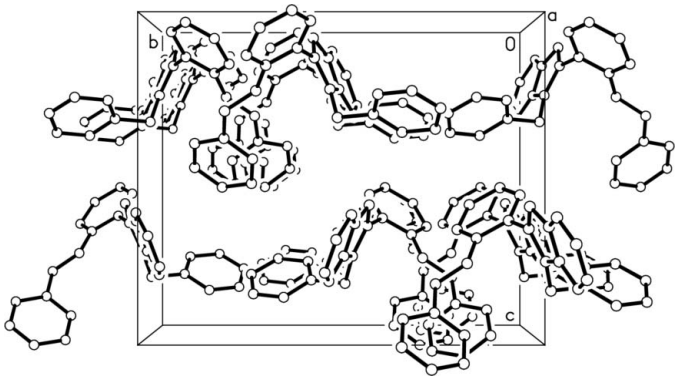


Figure 2
Perspective view of the crystal stacking pattern along the crystallographic *a* axis. For clarity, all H atoms have been omitted.

(Tong *et al.*, 2005; Elerman & Kabak, 1997), and metal complexes with Be^{II}, Co^{II} and Co^{III} (Tong *et al.*, 2005; Crane *et al.*, 1999). However, the benzimidazole and phenolate moieties are non-coplanar owing to the steric hindrance arising from effects of benzylation of the O- and N-atom positions. Thus, the dihedral angle between them increases to *ca* 72.2°, indicating that they are approximately perpendicular to each other, which is quite different from the coplanar conformation in 2-(2-hydroxyphenyl)benzimidazole, and 2-(1*H*-benzimidazol-2-yl)-6-methoxyphenol (Elerman & Kabak, 1997), but similar to the case of 2-(2-ethoxyphenyl)-1-ethyl-1*H*-benzimidazole, where the corresponding dihedral angle is *ca* 79° (Tong & Li, 2004).

The non-coplanarity, as well as the steric hindrances arising from the substituted benzyl groups at the O- and N-atom positions should also block the formation of the intermolecular π–π stacking interactions, which is in good agreement with the observation of no significant intermolecular π–π stacking interaction in the title compound. Moreover, no intermolecular C—H$\cdots\pi$ interaction can be found in the supramolecular array, which is in contrast to 2-(2-ethoxyphenyl)-1-ethyl-1*H*-benzimidazole (Tong & Li, 2004).

Furthermore, no intermolecular hydrogen bond interactions are observed. van der Waals interactions bind adjacent molecules in three dimensions (Fig. 2).

In conclusion, the observed weak photoluminescence for (I) is probably due to the non-coplanarity of the phenolate and benzimidazole moieties. In general, coplanarity enhances photoluminescent properties and deviation from coplanarity diminishes this. This is in agreement with the spectroscopic behavior of (I).

Experimental

The title compound was synthesized by a two-step reaction based on the method of Addison & Burke (1981). First, salicylic acid (0.138 g, 1 mmol) and *o*-phenylenediamine (0.108 g, 1 mmol) were mixed and stirred in syrupy phosphoric acid (3 ml) at a temperature of *ca* 520 K for 5 h to give white analytically pure 2-(2-hydroxyphenyl)benzimidazole after recrystallization of the crude product. The yield was *ca* 10%. Second, (I) was prepared by the reaction of 2-(2-hydroxyphenyl)benzimidazole (0.021 g, 0.1 mmol) and chloromethylbenzene (0.032 g, 0.2 mmol) under reflux in a yield of *ca* 70%. The X-ray quality single crystal used in the structure determination was grown by slow evaporation of an ethanol solution over several days. Analysis found: C 83.25, H 5.59, N 7.26%; calculated for $C_{27}H_{22}N_2O$: C 83.05, H 5.68, N 7.17%.

Crystal data

$C_{27}H_{22}N_2O$
M_r = 390.47
Orthorhombic, $Pna2_1$
a = 10.2724 (9) Å
b = 15.8390 (13) Å
c = 12.9779 (11) Å
V = 2111.6 (3) Å^3
Z = 4
D_x = 1.228 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2398 reflections
θ = 2.4–20.4°
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, colorless
0.53 × 0.33 × 0.28 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.979
11837 measured reflections
2400 independent reflections
2048 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.0°
$h = -13 \rightarrow 12$
$k = -20 \rightarrow 10$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.110
S = 1.08
2400 reflections
271 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.1914P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

The H atoms were placed at calculated positions in the riding-model approximation (C—H = 0.93 Å for aromatic H atoms, and 0.97 Å for methylene H atoms) with their displacement parameters tied to those of the parent atoms; $U_{iso}(H) = 1.2U_{eq}(C)$ for all aromatic and methylene H atoms.

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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References

Addison, A. W. & Burke, P. J. (1981). *J. Heterocycl. Chem.* **18**, 803–805.
Bruker. (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Crane, D. J., Sinn, E. & Tann, B. (1999). *Polyhedron*, **18**, 1527–1532.
Elerman, Y. & Kabak, M. (1997). *Acta Cryst.* C**53**, 372–374.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10, Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Svejda, P., Anderson, R. R. & Maki, A. H. (1978). *J. Am. Chem. Soc.* **100**, 7131–7138.
Tong, Y.-P. & Li, W. (2004). *Acta Cryst.* E**60**, o1563–o1565.
Tong, Y.-P., Zheng, S.-L. & Chen, X.-M. (2005). *Inorg. Chem.* **44**, 4270–4275.
Wu, T., Li, D., Feng, X. L. & Cai, J. W. (2003). *Inorg. Chem. Commun.* **6**, 886–890.