Ai-Ping Xing*, Dai Zeng, Shu-Ling Zhang, Jun-Jun Wei and Da-Feng Guo

Crystal structure of 2-((1H-benzo[d]imidazol-2-ylimino)methyl)-4,6-di-tert-butylphenol, C_{22}H_{27}N_{3}O.

Abstract
C_{22}H_{27}N_{3}O, monoclinic, P2_1/c (no. 14), a = 18.4984(4) Å, b = 11.4221(3) Å, c = 9.79600(19) Å, β = 90.9652(19)°, V = 2069.51(8) Å^3, Z = 4, R_{gt}(F) = 0.0605, wR_{ref}(F^2) = 0.1773, T = 293(2) K.

CCDC no.: 1900012

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material
In a typical experiment 2-aminobenzimidazole (1.3315 g, 10 mmol) and 3,5-bis(1,1-dimethylethyl)-2-hydroxybenzaldehyde (2.3433 g, 10 mmol) were mixed in 25 mL ethanol and refluxed for 3 h. When the solution was cooled to room temperature, a light yellow solid was obtained.

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Table 1: Data collection and handling.

<table>
<thead>
<tr>
<th>Crystal:</th>
<th>Yellow prism</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size:</td>
<td>0.2 × 0.15 × 0.13 mm</td>
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<tr>
<td>Wavelength:</td>
<td>Cu Kα radiation (1.54184 Å)</td>
</tr>
<tr>
<td>µ:</td>
<td>0.55 mm^-1</td>
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<tr>
<td>Diffractometer, scan mode:</td>
<td>Xcalibur, ω-scans</td>
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<tr>
<td>θ_{max}, completeness:</td>
<td>67°, &gt;99%</td>
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<tr>
<td>N(hkl)_measured, N(hkl)<em>unique, R</em>{int}:</td>
<td>18885, 3686, 0.049</td>
</tr>
<tr>
<td>Criterion for I_{obs}, N(hkl)_gt:</td>
<td>I_{obs} &gt; 2 σ(I_{obs}), 2825</td>
</tr>
<tr>
<td>Programs:</td>
<td>CrysAlisPRO [1], SHELX [2], OLEX2 [3]</td>
</tr>
</tbody>
</table>

Crystallization from methanol at room temperature gave the title compound as colorless crystals of good diffraction quality.

1H NMR (DMSO-d_6, 500 MHz) δ (p.p.m.): 13.34 (s, 1H), 12.79 (s, 1H), 9.63 (s, 1H), 7.67 (d, J = 2.4 Hz, 1H), 7.59 (s, 1H), 7.48 (d, J = 2.4 Hz, 2H), 7.23—7.18 (m, 2H), 1.44 (s, 9H), 1.31 (s, 9H).

13C NMR (DMSO-d_6, 126 MHz) δ (p.p.m.): 168.55, 158.54, 141.38, 136.54, 129.46, 129.37, 118.41, 35.15, 34.46, 31.65, 29.71.

IR (cm^-1, KBr): 3406 (br), 2906 (m), 2431 (m), 1910 (w), 1674 (s), 1603 (m), 1584 (m), 1513 (m), 1483 (m), 1452 (m), 1439 (m), 1397 (s), 1362 (w), 1320 (s), 1289 (s), 1249 (m), 1175 (s), 1072 (w), 1025 (w), 933 (m), 882 (w), 800 (m), 766 (w), 739 (w), 729 (m), 715 (s), 685 (w), 664 (w), 616 (w), 523 (m).

Experimental details
Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms. There is a disorder of one of the tert-butyl groups (Table 2, not shown in the figure).

Discussion
The structures of benzimidazole moiety have been widely studied, since they possess significant biological activity such as antitumor and antiproliferative [4, 5]. Schiff bases are also a very important family of the compounds because of their applications in biological and analytical chemistry [6—10]. The hybrid molecules composed by the combination of benzimidazole and Schiff base may exert potential biological...
activities. Thus we synthesized the Schiff base containing benzimidazole moiety.

The title compound crystallizes in the monoclinic system with a $P2_1/c$ space group with one $2\left[(1H$-benzo[d]imidazol-2-ylimino)methyl]-4,6-di-tert-butylphenol$ molecule in the asymmetric unit. As shown in the figure, the molecule structure consists of a 2,4-di-tert-butylphenol group and a benzimidazole group linked by the $-C\equiv N-$ group. The 2,4-di-tert-butylphenol ring is nearly planar excluding the methyl groups. The angle between two planes containing the benzimidazole ring/imine N atom and the phenol ring/imine C atom, respectively is 25.91°. The $C7$—N1 bonding distance of $2.860(2)$ Å forming an infinite chain.

### Acknowledgements
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### References
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