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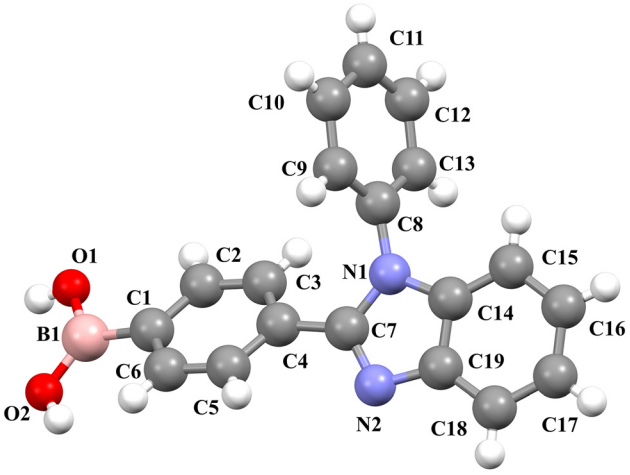
Crystal structure of (4-(1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)phenyl)boronic acid, $C_{19}H_{15}BN_2O_2$



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Abstract

$C_{19}H_{15}BN_2O_2$, triclinic, $P\bar{1}$ (no. 2), a = 6.0499(1) Å, b = 10.9750(3) Å, c = 12.6029(3) Å, α = 70.964(2)°, β = 87.736(2)°, γ = 79.962(2)°, V = 778.80(3) Å^3, Z = 2, $R_{gt}(F)$ = 0.0466, w$R_{ref}(F^2)$ = 0.1367, T = 293(2) K.

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The crystal structure is shown in the figure. Table 1 contains crystallographic data. The list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

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Table 1: Data collection and handling.

Crystal:	Clear light white bulk
Size:	0.03 × 0.02 × 0.01 mm
Wavelength:	CuKα radiation (1.54184 Å)
μ:	0.70 mm^{-1}
Diffractometer, scan mode:	XtaLAB Synergy, ω scans
θ_{max}, completeness:	73.9°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7,503, 2,984, 0.038
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2,578
$N(param)_{refined}$:	220
Programs:	Rigaku,[1] SHELX[2,3]

1 Source of materials

The mixture of 4-bromobenzoyl chloride (2.194 g, 10.00 mmol), N-phenylbenzene-1,2-diamine (1.842 g, 10.00 mmol), triethylamine (3 mL), and anhydrous tetrahydrofuran (THF, 30 mL) was stirred under an argon atmosphere. After 24 h, the reaction mixture was quenched with water (100 mL) and extracted with dichloromethane. Following solvent removal, the crude product was purified by recrystallization from a methanol-THF mixture, yielding a grey solid. This intermediate was then dissolved in acetic acid (10 mL) and heated to reflux for 12 h. After the acetic acid was evaporated, the resulting grey solid was identified as 4-(1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)phenyl) boronic acid, which was obtained in a yield of 71 %.

2 Experimental details

All hydrogen atoms were placed in idealized positions. Their U_{iso} values were set to 1.2U_{eq} of the parent atoms.

3 Comment

The 4-(1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)phenyl)boronic acid has emerged as a pivotal precursor in the fabrication of high-performance organic light-emitting diodes (OLEDs). Notably, Ken-Tsung Wong's work has demonstrated the utility of this

compound in the design of red phosphorescent OLEDs (PhOLEDs), utilizing 2,7-bis[4-(1-phenylbenzimidazol-2-yl) phenyl]-spirobifluorene as the electron-transporting host.[4] Moreover, Hans-Hermann Johannes and his collaborators have advanced the field by developing a series of styrene-functionalized monomers that incorporate phenylbenzo[d]imidazole units. These monomers, along with their corresponding homopolymers, exhibit remarkable thermal stability, as evidenced by their high glass-transition temperatures, which even exceed those of the widely employed electron-transporting material, 1,3,5-tris(1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzene (TPBI).[5]

The crystal structure of 4-(1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)phenylboronic acid is depicted in the figure above. The bond lengths of B1–C1, N1–C7, and N2=C7 in the title molecule are measured at 1.573 Å, 1.380 Å, and 1.321 Å, respectively, which are consistent with those observed in related analogs.[6,7] Additionally, the arrangement of adjacent molecules exhibits a parallel alignment, promoting π-π stacking interactions between the aromatic rings. All bond lengths and angles fall within the expected ranges, further confirming the structural integrity of the compound.[8]

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