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Crystal structure 1-cinnamyl-2-((*Z*)-styryl)-1*H*-benzo[*d*]imidazole – methanol (1/1), $C_{24}H_{20}N_2 \cdot CH_4O$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.29 × 0.25 × 0.21 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.07 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART, φ and ω -scans
$\theta_{\max}$, completeness:	25°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	12614, 3668, 0.031
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2498
$N(\text{param})_{\text{refined}}$:	257
Programs:	Bruker programmes [1], SHELX [2], OLEX2 [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.72290(18)	0.1877(3)	0.08352(15)	0.1369(10)
N1	0.53909(12)	0.3695(2)	0.09444(9)	0.0574(5)
N2	0.37855(11)	0.45544(18)	0.06166(8)	0.0500(4)
C1	0.52960(15)	0.5187(2)	0.11814(11)	0.0530(5)
C2	0.60172(17)	0.6120(3)	0.15585(12)	0.0665(6)
H2	0.66863(17)	0.5767(3)	0.17018(12)	0.0799(7)*
C3	0.57126(18)	0.7572(3)	0.17123(13)	0.0686(6)
H3	0.61847(18)	0.8215(3)	0.19653(13)	0.0824(8)*
C4	0.47197(17)	0.8114(3)	0.15020(12)	0.0627(6)
H4	0.45410(17)	0.9110(3)	0.16172(12)	0.0752(7)*
C5	0.39933(16)	0.7212(2)	0.11273(11)	0.0560(5)
H5	0.33276(16)	0.7576(2)	0.09822(11)	0.0672(6)*
C6	0.42996(14)	0.5742(2)	0.09767(10)	0.0492(5)
C7	0.44775(15)	0.3364(2)	0.06162(11)	0.0520(5)
C8	0.42310(16)	0.1910(2)	0.02675(11)	0.0578(5)
H8	0.46451(16)	0.1632(2)	−0.01009(11)	0.0693(7)*
C9	0.34846(16)	0.0941(2)	0.04165(11)	0.0559(5)
H9	0.34058(16)	0.0093(2)	0.01184(11)	0.0670(6)*
C10	0.27627(15)	0.1029(2)	0.09913(11)	0.0527(5)
C11	0.30036(17)	0.1784(3)	0.16308(11)	0.0605(6)
H11	0.36483(17)	0.2274(3)	0.17056(11)	0.0726(7)*
C12	0.2307(2)	0.1820(3)	0.21561(13)	0.0744(7)
H12	0.2478(2)	0.2343(3)	0.25804(13)	0.0893(8)*
C13	0.1365(2)	0.1092(3)	0.20577(16)	0.0894(8)
H13	0.0895(2)	0.1116(3)	0.24150(16)	0.1073(10)*
C14	0.1114(2)	0.0330(3)	0.14368(17)	0.0931(9)
H14	0.0468(2)	−0.0160(3)	0.13683(17)	0.1117(10)*
C15	0.18130(18)	0.0283(3)	0.09090(14)	0.0714(6)
H15	0.16404(18)	−0.0260(3)	0.04908(14)	0.0856(8)*
C16	0.27441(15)	0.4645(3)	0.02488(11)	0.0587(5)
H16a	0.27514(15)	0.5411(3)	−0.01252(11)	0.0705(7)*
H16b	0.25766(15)	0.3669(3)	0.00228(11)	0.0705(7)*

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Abstract

$C_{24}H_{20}N_2 \cdot CH_4O$, monoclinic, $P2_1/n$ (no. 14), $a = 12.764(3)$ Å, $b = 8.744(2)$ Å, $c = 18.733(5)$ Å, $\beta = 93.944(5)^\circ$, $V = 2085.8(9)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0501$, $wR_{\text{ref}}(F^2) = 0.1447$, $T = 296(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The 1-cinnamyl-2-((*E*)-styryl)-1*H*-benzo[*d*]methanol solvate (336 mg, 1 mmol) was dissolved in 20 mL of THF, and the

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C17	0.19095(15)	0.5039(3)	0.07357(12)	0.0601(6)
H17	0.19542(15)	0.4619(3)	0.11930(12)	0.0722(7)*
C18	0.11195(16)	0.5939(3)	0.05570(12)	0.0626(6)
H18	0.10944(16)	0.6330(3)	0.00946(12)	0.0751(7)*
C19	0.02687(15)	0.6409(3)	0.09930(12)	0.0616(6)
C20	0.02357(18)	0.6012(3)	0.17044(15)	0.0825(7)
H20	0.07411(18)	0.5353(3)	0.19117(15)	0.0990(9)*
C21	−0.0537(2)	0.6580(4)	0.21128(17)	0.0967(9)
H21	−0.0543(2)	0.6313(4)	0.25930(17)	0.1160(11)*
C22	−0.12910(19)	0.7534(4)	0.18125(18)	0.0920(9)
H22	−0.17993(19)	0.7940(4)	0.20905(18)	0.1104(10)*
C23	−0.12964(18)	0.7888(3)	0.11032(19)	0.0874(8)
H23	−0.18260(18)	0.8503(3)	0.08933(19)	0.1048(10)*
C24	−0.05243(17)	0.7339(3)	0.06987(14)	0.0742(7)
H24	−0.05335(17)	0.7598(3)	0.02168(14)	0.0891(8)*
C25	0.7943(3)	0.2165(5)	0.13800(19)	0.1312(14)
H25a	0.8078(17)	0.3245(6)	0.1406(10)	0.197(2)*
H25b	0.7678(10)	0.182(3)	0.1820(3)	0.197(2)*
H25c	0.8583(8)	0.163(3)	0.1302(8)	0.197(2)*
H1	0.6608(12)	0.215(3)	0.1007(15)	0.1574(16)*

solution was poured into the light of the reactor, which led to the N₂ protective gas. The reactor used a UV light of 365 nm as the light source and air cooling. The reaction was complete within 6 h (TLC detection). Then removing the solvent under vacuum gave the crude product, which was then recrystallized with EA/hexane (10–15%) to afford the 1-cinnamyl-2-((*Z*)-styryl)-1*H*-benzo[*d*]imidazole solid. Yield, 302 mg, 90%. The title compound (67 mg, 0.2 mmol) was dissolved in 20% EA/Hex, and the solvent slowly evaporated at room temperature. After four days, colorless crystals were obtained.

Experimental details

Using Olex2, [1] the structure was solved with the SHELXS package [2, 3]. All of the hydrogen atoms were placed in the calculated positions and all the non-hydrogen atoms were refined anisotropically.

Discussion

The 1,2-disubstituted benzimidazole compounds have potential applications in synthetic chemistry [4–6] and medicinal

chemistry [7–9]. The NMR results are consistent with the proposed structure. The bond lengths and angles in the title molecule (*cf.* the figure) are in the normal ranges. In conclusion, an efficient and green one-step approach to the title compound has been developed.

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