Shi-Jun Chen, Hao Zhu, Meng-Meng Zhang, Wen-Wu Xu, Yu-Cai Wang and Zhi-Fei Zhang*

Crystal structure of 1-benzyl-3-cyano-6-phenyl-1,2-dihydropyridine, C₁₉H₁₆N₂

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.25 × 0.20 × 0.18 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.07 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	26.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9396, 2961, 0.024
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2480
$N(\text{param})_{\text{refined}}$:	190
Programs:	Bruker [1], SHELX [2, 3]

and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

Phenylmagnesium bromide (3.77 g, 24 mmol), bromobenzene (0.56 g, 3.5 mmol), and magnesium (0.55 g, 23 mmol) were added to 1-benzyl-3-cyanopyridine bromide (5.50 g, 20 mmol) [4–6]. Stirring was continued for 20 min with cooling to room temperature. The solution was washed three times with water to obtain a mixture. After drying of the organic layer over sodium sulfate the solution was filtered and evaporated to dryness. The resulting oil was purified by silica gel column chromatography using a mixture of petroleum ether and ethyl acetate. Finally, the resulting solution was evaporated to dryness in vacuo to give the title compound as colorless crystals.

Experimental details

All hydrogen atoms were placed in the calculated positions and all the non-hydrogen atoms were refined anisotropically.

Comment

In recent years, it was reported that the title compound is a estrogen receptor [7]. Estrogen receptors are more abundant in the cells of the target organs, and can specifically bind to hormones to form hormone-receptor complexes, allowing hormones to exert their biological effects. This may be important in the treatment of cancer, cardiovascular disease, inflammatory disease, immune and reproductive systems [8–10].

The title compound crystallize in the orthorhombic crystal system with the space group of $P2_12_12_1$. When a pyridine

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Abstract

C₁₉H₁₆N₂, orthorhombic, $P2_12_12_1$ (no. 19), $a = 7.5177(10)$ Å, $b = 12.4761(16)$ Å, $c = 16.118(2)$ Å, $V = 1511.7(3)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0424$, $wR_{\text{ref}}(F^2) = 0.0967$, $T = 293(2)$ 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

***Corresponding author: Zhi-Fei Zhang**, School of Pharmacy, North China University of Science and Technology, 063210 Caofeidian District, Tangshan, P.R. China, e-mail: zhangzhifeifei7208@163.com

Shi-Jun Chen, Meng-Meng Zhang and Wen-Wu Xu: School of Pharmacy, North China University of Science and Technology, 063210 Caofeidian District, Tangshan, P.R. China

Hao Zhu: School of Public Health, North China University of Science and Technology, 063210 Caofeidian District, Tangshan, P.R. China

Yu-Cai Wang: Jia Mu Si University, School of Continuing Education, No.148 Xuefu St, Jiamusi, Heilongjiang, P.R. China

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

Atom	x	y	z	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C1	0.4955(3)	0.3905(2)	0.67032(15)	0.0460(6)
C2	0.3887(4)	0.3378(3)	0.7272(2)	0.0645(8)
H2	0.3774	0.3645	0.7808	0.077*
C3	0.2992(5)	0.2462(3)	0.7048(3)	0.0833(11)
H3	0.2265	0.2121	0.7433	0.100*
C4	0.3153(5)	0.2049(3)	0.6274(3)	0.0839(12)
H4	0.2546	0.1427	0.6130	0.101*
C5	0.4211(4)	0.2551(3)	0.5709(2)	0.0710(9)
H5	0.4326	0.2267	0.5178	0.085*
C6	0.5119(4)	0.3482(2)	0.59167(17)	0.0539(7)
H6	0.5837	0.3820	0.5526	0.065*
C7	0.5836(4)	0.4947(2)	0.69547(18)	0.0573(7)
H7A	0.4974	0.5523	0.6912	0.069*
H7B	0.6200	0.4897	0.7531	0.069*
C8	0.7268(4)	0.5986(2)	0.58754(18)	0.0537(7)
H8	0.6280	0.6434	0.5871	0.064*
C9	0.8543(4)	0.6140(2)	0.53020(17)	0.0566(7)
C10	1.0007(4)	0.5388(2)	0.52736(17)	0.0594(7)
H10	1.0825	0.5427	0.4842	0.071*
C11	1.0196(4)	0.4646(2)	0.58515(16)	0.0562(7)
H11	1.1095	0.4140	0.5791	0.067*
C12	0.9021(3)	0.4587(2)	0.66022(16)	0.0487(6)
H12	0.8688	0.3835	0.6683	0.058*
C13	0.8407(4)	0.6955(3)	0.4693(2)	0.0726(9)
C14	0.9961(3)	0.4968(2)	0.73890(15)	0.0460(6)
C15	0.9761(4)	0.4442(3)	0.81351(18)	0.0650(8)
H15	0.9055	0.3831	0.8167	0.078*
C16	1.0619(5)	0.4825(4)	0.88418(19)	0.0827(11)
H16	1.0483	0.4470	0.9345	0.099*
C17	1.1660(5)	0.5721(3)	0.8799(2)	0.0781(10)
H17	1.2212	0.5978	0.9276	0.094*
C18	1.1894(4)	0.6241(3)	0.8064(2)	0.0656(8)
H18	1.2619	0.6844	0.8038	0.079*
C19	1.1055(3)	0.5874(2)	0.73565(17)	0.0509(6)
H19	1.1218	0.6231	0.6856	0.061*
N1	0.7358(3)	0.52085(16)	0.64567(14)	0.0488(5)
N2	0.8327(5)	0.7609(3)	0.4197(2)	0.1090(12)

has one electron-withdrawing substituent at the 3 position or two such substituents at the 3 and 5 positions the reaction proceeds faster, forming a cyanopyridine salt which is

then reacted with phenylmagnesium bromide to give the title product. However, due to the steric hindrance effect, the phenyl groups are arranged side by side. In the crystal structure, several important bond angles are as follows C8–N1–C7 = 120.7(2)°, C8–N1–C12 = 121.7(2)°, C7–N1–C12 = 117.6(2)°, C11–C12–C14 = 112.6(2)°. Generally all bond lengths and angles are in the expected ranges.

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