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The crystal structure of 5-bromo-2-(1-methyl-1*H*-tetrazol-5-yl)pyridine, C₇H₆BrN₅

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Abstract

C₇H₆BrN₅, orthorhombic, *Acam* (no. 64; unconventional setting of *Cmce* formerly known as *Cmca*), $a = 12.3735(8)$ Å, $b = 20.8690(11)$ Å, $c = 6.8385(6)$ Å, $V = 1765.9(2)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0471$, $wR_{\text{ref}}(F^2) = 0.1152$, $T = 293(2)$ K.

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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.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.28 × 0.25 × 0.23 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	4.61 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, ω
θ_{max} , completeness:	29.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3550, 1181, 0.062
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 850
$N(\text{param})_{\text{refined}}$:	80
Programs:	CysAlis ^{PRO} [1], SHELX [2, 3]

Source of material

The title compound was synthesized according to a reported procedure [4]. 5-Bromo-2-(2*H*-tetrazol-5-yl)pyridine was reacted with sodium azide and ammonium chloride in DMF at 120 °C for 1 h. The addition of iodomethane to the solution of 5-bromo-2-(2*H*-tetrazol-5-yl)pyridine in dry DMF produced a mixture of 5-bromo-2-(1-methyl-1*H*-tetrazol-5-yl)pyridine and 5-bromo-2-(2-methyl-2*H*-tetrazol-5-yl)pyridine at room temperature. The title compound was separated by silica-gel column chromatography using a gradient of ethyl acetate/petroleum ether (10–20%). Crystals were obtained by slow evaporation of mixed solution of petroleum ether and ethyl acetate (5:1, v/v) at room temperature after a week.

Experimental details

Hydrogen atoms were situated in idealized positions with the carrier atom-H distances = 0.93 Å for aryl, 0.97 Å for methyl.

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.16881(4)	0.05998(2)	0.5000	0.0488(2)
C1	0.3491(4)	−0.0243(2)	0.5000	0.0376(11)
H1	0.3886	0.0136	0.5000	0.045*
C2	0.2377(3)	−0.0206(2)	0.5000	0.0346(10)
C3	0.1778(3)	−0.0761(3)	0.5000	0.0413(12)
H3	0.1027	−0.0748	0.5000	0.050*
C4	0.2321(3)	−0.1337(2)	0.5000	0.0391(11)
H4	0.1941	−0.1722	0.5000	0.047*
C5	0.3436(3)	−0.1336(2)	0.5000	0.0323(10)
C6	0.3998(4)	−0.1953(2)	0.5000	0.0358(10)
N1	0.4026(3)	−0.07970(19)	0.5000	0.0369(9)
N2	0.5064(3)	−0.20657(17)	0.5000	0.0387(9)
N3	0.5218(3)	−0.2707(2)	0.5000	0.0519(11)
N4	0.4272(4)	−0.2963(2)	0.5000	0.0591(13)
N5	0.3493(3)	−0.2510(2)	0.5000	0.0513(12)
C7	0.6007(4)	−0.1639(3)	0.5000	0.0562(15)
H7A ^a	0.6643	−0.1881	0.5314	0.084*
H7B ^a	0.5905	−0.1308	0.5957	0.084*
H7C ^a	0.6088	−0.1449	0.3730	0.084*

^aOccupancy: 0.5.

The U_{iso} values of the hydrogen atoms of methyl groups were set to $1.5U_{\text{eq}}$ and the U_{iso} values of all other hydrogen atoms were set to $1.2U_{\text{eq}}$ (C).

Comment

Tetrazole, an important five-membered heterocycle, is well employed in medicinal chemistry due to its *N*-donor characteristics. Tetrazole derivatives have been reported to possess a broad spectrum of biological activities, such as antibacterial [5, 6], anticancer [7, 8], anti-Alzheimer's disease [9, 10], antitubercular [11, 12], antimalarial [13, 14], and antifungal [15, 16] properties. Moreover, many tetrazole-based drugs such as Tedizolid, Cilostazol, Cefamandole and Irbesartan have already been used in clinical practice for the treatment of various diseases. Demonstrating the therapeutic potential of tetrazole derivatives. Here we report the crystal structure of the title compound to expect a better understanding of this structure.

The title compound crystallizes with one half of a molecule in the asymmetric unit (*cf.* the figure). The bond lengths of Br1—C2 is 1.885(3) Å. The distances between N1 and N2 is 2.942(7) Å. Interestingly, not only pyridine ring and tetrazole ring are coplanar but also methyl group and the N atom of pyridine are on the same side. Geometric parameters are in expected ranges [17].

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