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The crystal structure of 4-(3-bromophenyl)pyrimidin-2-amine, $C_{10}H_8BrN_3$

<https://doi.org/10.1515/ncrs-2021-0176>

Received May 9, 2021; accepted May 31, 2021;

published online June 18, 2021

Abstract

$C_{10}H_8BrN_3$, orthorhombic, *Pbca* (no. 61), $a = 7.214(3)$ Å, $b = 12.735(6)$ Å, $c = 21.305(9)$ Å, $V = 1957.3(15)$ Å³, $Z = 8$, $R_{gt}(F) = 0.0353$, $wR_{ref}(F^2) = 0.0808$, $T = 293$ K.

CCDC no.: 2081364

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:	Colorless needle
Size:	0.20 × 0.10 × 0.10 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	4.16 mm ⁻¹
Diffractometer, scan mode:	D8/Apex2, φ and ω
θ_{max} , completeness:	27.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	8521, 2104, 0.074
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1295
$N(param)_{refined}$:	148
Programs:	Bruker [1], SHELX [2], Diamond [3]

Source of material

The target compound was synthesized according to the reported protocol [4]. Single crystals of diffraction quality are obtained by slow evaporation of the acetone solvent after three days.

Experimental details

Some hydrogen atoms were placed in calculated positions; others that were seen in the difference Fourier map and refined freely (Table 2).

Comment

Pyrimidine is a class of heterocyclic compounds characterized by the presence of three carbon and two nitrogen atoms in the ring. Pyrimidine functionalized compounds are of medicinal value and possess diverse range of bioactivities [5–7]. Besides its medicinal potential, it also found application in the field material chemistry towards light harvesting devices [8] and molecular wires [9].

There is one molecule in the asymmetric unit (see the Figure), and the geometric parameters are in the expected ranges [10]. The molecules in the crystal are associated through $N3-H3A \cdots N1$ (2.21 Å), $N3-H3B \cdots N2$ (2.19 Å), hydrogen bonds forming a sheet structure along. Weak $\pi-\pi$ interactions also exist between benzene rings of two

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

Atom	x	y	z	U _{iso} [*] /U _{eq}
Br1	1.15001 (5)	0.31066 (3)	0.30008 (2)	0.07590 (19)
N1	0.5385 (3)	0.35611 (14)	0.43861 (9)	0.0361 (5)
N2	0.2294 (3)	0.38830 (15)	0.47474 (10)	0.0390 (5)
N3	0.3831 (4)	0.23631 (19)	0.49909 (13)	0.0524 (7)
C1	0.9874 (4)	0.4209 (2)	0.32252 (12)	0.0480 (7)
C2	1.0311 (4)	0.5225 (2)	0.30664 (12)	0.0577 (8)
H2	1.1362	0.5375	0.2830	0.069*
C3	0.9152 (4)	0.6018 (3)	0.32674 (16)	0.0642 (9)
C4	0.7563 (4)	0.5799 (2)	0.36060 (15)	0.0531 (8)
C5	0.7124 (3)	0.47727 (19)	0.37535 (12)	0.0371 (6)
C6	0.8305 (3)	0.3979 (2)	0.35617 (11)	0.0416 (6)
H6	0.8033	0.3285	0.3662	0.050*
C7	0.5414 (3)	0.45067 (17)	0.41095 (11)	0.0347 (6)
C8	0.3901 (4)	0.5168 (2)	0.41544 (13)	0.0425 (7)
C9	0.2387 (4)	0.48138 (19)	0.44723 (13)	0.0430 (6)
H9	0.1357	0.5251	0.4498	0.052*
C10	0.3840 (3)	0.33006 (18)	0.47004 (12)	0.0365 (6)
H3	0.953 (4)	0.678 (2)	0.3179 (14)	0.065 (9)*
H4	0.678 (3)	0.634 (2)	0.3768 (11)	0.039 (7)*
H8	0.392 (3)	0.578 (2)	0.3995 (11)	0.040 (7)*
H3A	0.289 (4)	0.216 (2)	0.5200 (14)	0.055 (9)*
H3B	0.477 (4)	0.1975 (18)	0.4994 (13)	0.048 (9)*

adjacent molecules which also assist in the overall construction of the crystal structure.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: This research was financially supported by the National Key Research and Development Program of

China (2017YFA0205301), NSFC (61701176), Taif University Researches Supporting Project number (TURSP-2020/01), Taif University, Taif, Saudi Arabia.

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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