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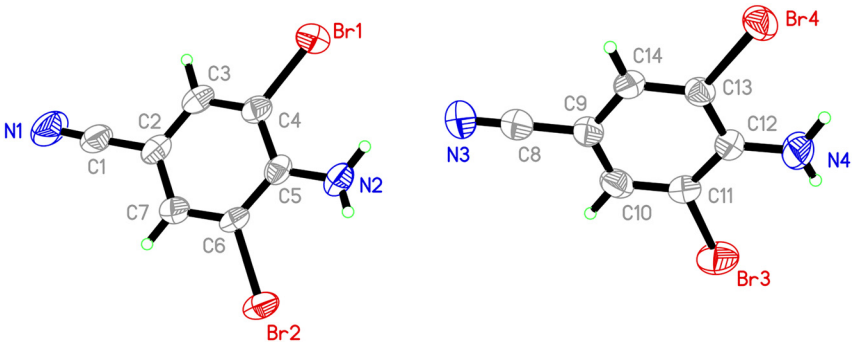
Crystal structure of 4-amino-3,5-dibromobenzonitrile, $C_7H_4Br_2N_2$



https://doi.org/10.1515/ncrs-2024-0068
Received February 16, 2024; accepted March 20, 2024;
published online April 5, 2024

Abstract

$C_7H_4Br_2N_2$, monoclinic, $C2/c$ (no. 15), a = 42.364(10) Å, b = 3.9052(4) Å, c = 23.783(3) Å, β = 120.984(9)°, V = 3373.2(10) Å^3, Z = 16, $R_{gt}(F)$ = 0.0415, $wR_{ref}(F^2)$ = 0.1073, T = 298 K.

CCDC no.: 2333289

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.

1 Source of materials

The title molecule 4-amino-3,5-dibromobenzonitrile (**4ADBN**) (0.275 g, 1 mmol) was obtained commercially and recrystallized from 15 mL *n*-hexane/CH_2Cl_2 (*v*/*v*, 2/1) solution. After dissolving fully for several minutes, the precursor solution was maintained at room temperature to obtain some crystals in the form of block.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.10 × 0.08 × 0.08 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	11.7 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	63.8°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	13,549, 2783, 0.074
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2435
$N(param)_{refined}$:	212
Programs:	Bruker [1], SHELX [2, 4], Olex2 [3], Diamond [5]

2 Experimental details

The structure of crystal was solved by SHELXT [2] program within Olex2 [3] and refined by SHELXL [4]. The graphics were finished using Diamond [5].

3 Comment

The asymmetric unit of title compound consists of two **4ADBN** molecules and these are not in the same plane. There is one hydrogen bond, N–H···N, the angle of N–H···N is 145(5)°, the distance of H···N is 2.19(7) Å between two **4ADBN** molecules of asymmetric unit. The bond distances of Br1–C4, Br2–C6, Br3–C11, Br4–C13 are 1.904(5) Å, 1.898(4) Å, 1.887(5) Å, 1.904(4) Å being in normal range of the literature [6–8]. At the same time, different **4ADBN**s are interacted by various

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.19998 (2)	0.81994 (18)	0.40496 (3)	0.0562 (2)
Br2	0.19314 (2)	0.36704 (15)	0.17152 (3)	0.0505 (2)
Br3	0.44836 (2)	0.60720 (18)	0.49515 (3)	0.0630 (2)
Br4	0.44155 (2)	0.01878 (17)	0.70798 (2)	0.0508 (2)
N1	0.04755 (14)	0.9185 (19)	0.1478 (3)	0.0812 (19)
C1	0.07803 (15)	0.8492 (16)	0.1751 (3)	0.0527 (14)
C2	0.11608 (13)	0.7614 (14)	0.2112 (2)	0.0424 (11)
C3	0.13671 (13)	0.8210 (13)	0.2784 (3)	0.0426 (11)
H3	0.125816	0.922219	0.299695	0.051*
C4	0.17312 (13)	0.7298 (13)	0.3132 (2)	0.0386 (11)
C5	0.19138 (12)	0.5848 (12)	0.2840 (2)	0.0379 (11)
N2	0.22760 (12)	0.5014 (15)	0.3192 (3)	0.0539 (12)
H2A	0.2402 (17)	0.491 (16)	0.363 (3)	0.065*
H2B	0.2362 (17)	0.375 (17)	0.305 (3)	0.065*
C6	0.16994 (12)	0.5410 (12)	0.2158 (2)	0.0358 (10)
C7	0.13323 (13)	0.6215 (14)	0.1796 (2)	0.0426 (12)
H7	0.119904	0.583461	0.134614	0.051*
N3	0.29244 (14)	0.347 (2)	0.4507 (3)	0.085 (2)
C8	0.32347 (16)	0.3304 (17)	0.4820 (3)	0.0555 (15)
C9	0.36289 (14)	0.3235 (14)	0.5207 (2)	0.0447 (12)
C10	0.38371 (14)	0.4413 (14)	0.4952 (2)	0.0460 (12)
H10	0.372043	0.521023	0.452244	0.055*
C11	0.42146 (14)	0.4417 (14)	0.5327 (2)	0.0424 (11)
C12	0.44044 (13)	0.3172 (13)	0.5973 (2)	0.0402 (11)
N4	0.47746 (12)	0.3147 (17)	0.6345 (2)	0.0630 (14)
H4A	0.4878 (14)	0.275 (19)	0.6754 (12)	0.076*
H4B	0.4913 (13)	0.395 (17)	0.622 (3)	0.076*
C14	0.38043 (13)	0.1947 (14)	0.5843 (2)	0.0411 (11)
H14	0.366769	0.110094	0.601784	0.049*
C13	0.41827 (12)	0.1943 (12)	0.6209 (2)	0.0359 (10)

weak interactions, such as hydrogen bonds, N–H···Br, N–H···N, C–H···Br and π···π, existing in packing structure.

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

Research funding: None declared.

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

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