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Crystal structure of 3-aminopyrazine-2-carbohydrazide, C₅H₇N₅O

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Abstract

C₆H₈N₄O, monoclinic, $P2_1/c$ (no. 14), $a = 10.1022(8)$ Å, $b = 9.4818(8)$ Å, $c = 7.0832(6)$ Å, $\beta = 94.1380(10)^\circ$, $V = 676.71(10)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0357$, $wR_{\text{ref}}(F^2) = 0.1088$, $T = 296(2)$ K.

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The asymmetric unit of the title 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 title compound was synthesized via methyl 3-aminopyrazine-2-carboxylate (1 mmol) with excess hydrazine hydrate (4 mmol) in methanol solution (5 mL) under refluxing. The crystal suitable for single X-ray diffraction was obtained by recrystallization from acetonitrile solution.

Experimental details

The structure was solved by direct methods and refined with the SHELX crystallographic software package [1]. The

Table 1: Data collection and handling.

Crystal:	Colourless rod
Size:	0.20 × 0.07 × 0.06 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.11 mm ⁻¹
Diffractometer, scan mode:	CCD area detector, φ and ω
θ_{max} , completeness:	25.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3368, 1189, 0.014
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1031
$N(\text{param})_{\text{refined}}$:	108
Programs:	SHELX [1], Bruker [2]

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	0.58410(12)	1.00465(11)	0.2509(2)	0.0583(4)
C1	0.84077(15)	0.61084(17)	0.1383(2)	0.0440(4)
H1	0.848540	0.513108	0.140645	0.053*
C2	0.94451(16)	0.69136(18)	0.0840(2)	0.0445(4)
H2	1.021405	0.645852	0.052358	0.053*
C3	0.82726(14)	0.89406(16)	0.1202(2)	0.0371(4)
C4	0.72119(13)	0.81064(15)	0.18054(19)	0.0333(4)
C5	0.59630(14)	0.87579(15)	0.2387(2)	0.0372(4)
N1	0.72925(12)	0.67097(13)	0.18749(18)	0.0391(4)
N2	0.94009(12)	0.83034(14)	0.07467(19)	0.0426(4)
N3	0.82308(14)	1.03440(14)	0.1044(2)	0.0516(4)
H3A	0.890211	1.079453	0.066743	0.062*
H3B	0.753256	1.079695	0.131829	0.062*
N4	0.50134(12)	0.78739(13)	0.2785(2)	0.0415(4)
H4	0.515859	0.698181	0.272567	0.050*
N5	0.37589(14)	0.83521(15)	0.3307(3)	0.0512(4)
H5A	0.390(2)	0.875(2)	0.4432(16)	0.078(7)*
H5B	0.349(2)	0.894(2)	0.241(2)	0.101(9)*

hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Comment

Pyrazine hydrazones and their metal complexes have been paid much attention primarily due to the excellent pharmacological activities [3]. As part of our continuous work on pyrazine derivative [4], the title compound was synthesized and its crystal structure is presented here.

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In the title structure (*cf.* the figure), the bond length of C=O double bonds are 1.2317(18) Å, comparable with the literature values [5–7]. All other molecular geometric parameters are in the expected ranges. In the crystal, a pair of classical intermolecular N–H···N hydrogen bonds between the amino and pyrazine N atoms link two adjacent molecules into a centrosymmetry dimer. The dimers are connected with each other via intermolecular N–H···O hydrogen to form a two-dimensional.

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