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Crystal structure of 5-methylpyrazine-2-carbohydrazide, C₆H₈N₄O

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.15 × 0.12 × 0.12 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.1 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART, φ and ω -scans
$\theta_{\max}$, completeness:	25°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3475, 1264, 0.020
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1058
$N(\text{param})_{\text{refined}}$:	108
Programs:	Bruker programs [1], SHELX [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	0.53440(16)	0.28260(12)	0.19381(13)	0.0557(4)
N1	0.28756(17)	0.01491(13)	0.02094(15)	0.0423(4)
N2	0.12418(18)	0.22765(14)	−0.14170(16)	0.0483(4)
N3	0.51085(17)	0.07141(14)	0.27442(15)	0.0436(4)
H3	0.456811	−0.003076	0.262270	0.052*
N4	0.6435(2)	0.08473(17)	0.39527(18)	0.0548(5)
H4A	0.600(3)	0.120(2)	0.4685(19)	0.074(7)*
H4B	0.706(3)	0.148(2)	0.367(3)	0.104(10)*
C1	0.1653(2)	−0.00347(17)	−0.09352(18)	0.0443(4)
H1	0.132935	−0.090753	−0.119462	0.053*
C2	0.0829(2)	0.10085(17)	−0.17678(18)	0.0406(4)
C3	0.2481(2)	0.24671(17)	−0.02734(18)	0.0444(4)
H3A	0.280247	0.333889	−0.000652	0.053*
C4	0.3302(2)	0.14228(15)	0.05256(17)	0.0370(4)
C5	0.4676(2)	0.17114(15)	0.17919(17)	0.0383(4)
C6	−0.0542(2)	0.07644(19)	−0.3054(2)	0.0543(5)
H6A	−0.071441	−0.018139	−0.318802	0.081*
H6B	−0.156734	0.117503	−0.285243	0.081*
H6C	−0.022335	0.114331	−0.394668	0.081*

<https://doi.org/10.1515/ncrs-2018-0187>

Received May 25, 2018; accepted July 9, 2018; available online July 20, 2018

Abstract

C₆H₈N₄O, monoclinic, $P2_1/c$ (no. 14), $a = 8.019(5)$ Å, $b = 9.990(6)$ Å, $c = 9.050(6)$ Å, $\beta = 98.474(10)^\circ$, $V = 717.1(7)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0405$, $wR_{\text{ref}}(F^2) = 0.1205$, $T = 296(2)$ K.

CCDC no.: 1854561

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 5-methylpyrazine-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.

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Experimental details

The structure was solved by Direct Methods and refined with the SHELX crystallographic software package [2]. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Discussion

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 derivatives [4], the title compound was synthesized and its crystal structure is presented here.

There is one molecule in the asymmetric unit (*cf.* the figure). In the title compound, the bond length of the C=O double bond is 1.234(2) Å, comparable with the literature values [5]. Bond lengths and angles are comparable with those found in the crystal structure of a directly related pyrazine carboxy compound [6]. In the crystal, intermolecular N—H···O hydrogen bonds link the molecules into a chain-like structure along *b* axis.

References

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