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The crystal structure of (2*E*,2'*E*)-,2,2'-bis[1-(2-pyrazinyl)ethylidene]carbonimidic dihydrazide, C₁₃H₁₅N₉

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.35 × 0.32 × 0.30 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.09 mm ⁻¹
Diffractometer, scan mode:	Bruker diffractometer, ω
$\theta_{\max}$, completeness:	25.0°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6922, 2492, 0.021
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1898
$N(\text{param})_{\text{refined}}$:	209
Programs:	Bruker [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>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.07590(7)	0.5390(2)	1.09893(11)	0.0575(5)
N2	0.17449(6)	0.55003(19)	1.01583(9)	0.0410(4)
N3	0.15960(6)	0.71885(19)	0.85094(10)	0.0407(4)
N4	0.21547(6)	0.66258(19)	0.87918(9)	0.0410(4)
H4	0.224282	0.618378	0.928615	0.049*
N5	0.24357(7)	0.7678(2)	0.75604(10)	0.0479(4)
H5A	0.269179	0.779267	0.722338	0.057*
H5B	0.209181	0.814061	0.743976	0.057*
N6	0.31019(6)	0.6085(2)	0.84405(9)	0.0400(4)
N7	0.31724(6)	0.52098(19)	0.91946(9)	0.0376(4)
N8	0.43300(6)	0.3134(2)	1.05402(11)	0.0494(4)
N9	0.33964(8)	0.2675(2)	1.14515(11)	0.0546(5)
C1	0.07366(8)	0.6099(3)	1.02324(13)	0.0507(5)
H1	0.037925	0.656515	0.997631	0.061*
C2	0.12781(9)	0.4726(3)	1.13238(13)	0.0508(5)
H2	0.131330	0.420084	1.184910	0.061*
C3	0.17647(8)	0.4795(3)	1.09145(12)	0.0457(5)
H3	0.212046	0.432940	1.117730	0.055*
C4	0.12249(7)	0.6178(2)	0.98010(11)	0.0371(4)
C5	0.11788(7)	0.6974(2)	0.89628(12)	0.0409(5)
C6	0.05817(9)	0.7622(3)	0.85571(16)	0.0580(6)
H6A	0.0455(11)	0.854(3)	0.8951(17)	0.087*
H6B	0.0616(11)	0.812(3)	0.8010(19)	0.087*
H6C	0.0266(12)	0.665(3)	0.8449(17)	0.087*
C7	0.25724(7)	0.6779(2)	0.82724(11)	0.0367(4)
C8	0.41925(8)	0.4661(3)	0.89180(13)	0.0535(5)

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Abstract

C₁₃H₁₅N₉, monoclinic, *C*2/*c* (no. 15), *a* = 22.827(5) Å, *b* = 7.8830(16) Å, *c* = 16.020(3) Å, β = 98.95(3)°, *V* = 2847.6(10) Å³, *Z* = 8, *R*_{gt}(*F*) = 0.0416, *wR*_{ref}(*F*²) = 0.1331, *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.

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H8A	0.453143	0.407350	0.921172	0.080*
H8B	0.407531	0.415281	0.837311	0.080*
H8C	0.429191	0.583094	0.884865	0.080*
C9	0.36906(7)	0.4548(2)	0.94187(11)	0.0372(4)
C10	0.37833(7)	0.3673(2)	1.02363(11)	0.0372(4)
C11	0.33207(8)	0.3393(3)	1.06992(12)	0.0480(5)
H11	0.294024	0.372938	1.046402	0.058*
C12	0.39494(10)	0.2218(3)	1.17591(14)	0.0578(6)
H12	0.402847	0.175318	1.229849	0.069*
C13	0.44041(10)	0.2413(3)	1.13035(14)	0.0587(6)
H13	0.477970	0.202919	1.153442	0.070*

Source of material

The mixture of 1-(pyrazin-2-yl)ethanone 24.2 mg, 0.2 mmol and carbonimidic dihydrazide 8.9 mg (0.1 mmol) was dissolved in 5 mL methanol and acetonitrile and stirred for 15 minutes. The mixture was transferred to the autoclave lined with PTFE and heated at 180 °C for 16 hours. Then the temperature was reduced to 120 °C and heated for 6 hours, and finally reduced to room temperature. Light yellow crystals were obtained.

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.

Comment

There is a need for the development of new drugs to treat cancer due to the recent and rapid appearance of numerous single, multiple, and extensively drug-resistant forms of the disease [3, 4]. Therefore, the search for highly efficient and safe antitumor agents has become more urgent than ever before. The aminoguanidine class [6–11], a diverse group of bioactive compounds used in the treatment of a broad range of diseases from bacterial infections to cancer and diabetes are already approved for human use.

The asymmetric unit of the title structure contains one title molecule. The bond lengths and angles within these moieties are in the expected ranges [12]. The N(1)–C(1), N(1)–C(2), N(2)–C(3), N(2)–C(4), N(3)–C(5), N(3)–N(4) and N(4)–C(7) bonds are 1.327(6) Å, 1.337(6) Å, 1.330(5) Å, 1.348(5) Å, 1.369(2) Å, 1.294(5) Å and 1.359(5) Å in the range of the typical C=N double bond. The dihedral angles between the C10–C11–N9–C12–C13–N8 pyrazine ring and the second

pyrazine ring C1–C4–N2–C3–C2–N1 is 4.7°. It is possible that the two pyrazine rings are not completely coplanar due to repulsive forces between molecules.

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