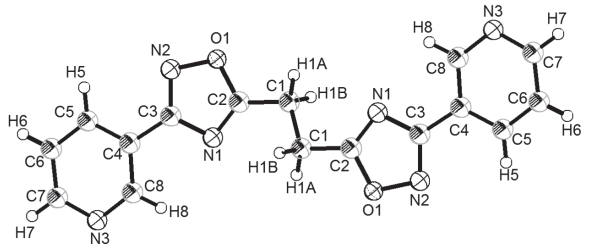
Fei Liu*, Huang Fang, Fang Zhang and Qifan Chen

The crystal structure of 1,2-bis(3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl)ethane, $C_{16}H_{12}N_6O_2$



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Abstract

$C_{16}H_{12}N_6O_2$, monoclinic, $P2_1/c$ (no. 14), $a = 4.791(5)$ Å, $b = 28.156(5)$ Å, $c = 5.747(5)$ Å, $\beta = 109.941(5)°$, $V = 728.8(10)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0407$, $wR_{ref}(F^2) = 0.0998$, $T = 293(2)$ K.

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The 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

N-hydroxy-nicotinamidine is easily available by a literature known synthesis [3]. A mixture of *N*-hydroxy-nicotinamidine (0.04 mol) and succinic anhydride (0.08 mol) was heated to 428 K and kept at this temperature for 4 h. The reaction mixture was cooled to room temperature, and washed with water. A solution (15 mL) of methanol was added. The mixture was shocked at ultrasonic and washed with a solution of sodium hydroxide (1 M, 10 mL). The pH value of the solution was adjusted to three. The suspension was filtered. The filter residue was washed with water, recrystallized from ethanol, dissolved with methanol, filtered, and was allowed to diffuse slowly into the solution of the filtrate. Colourless crystals were obtained in about 4 weeks.

Table 1: Data collection and handling.

Crystal:	Block, colourless
Size:	0.21 × 0.17 × 0.15 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.10 mm^{-1}
Diffractometer, scan mode:	Bruker FRAMBO, φ and ω-scans
$2\theta_{max}$, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	2228, 1282, 0.019
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 955
$N(param)_{refined}$:	109
Programs:	Bruker programs [1], SHELX [2]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
N1	0.3221(3)	0.07196(5)	0.7006(3)	0.0411(4)
N2	0.5881(3)	0.08333(5)	1.1033(3)	0.0513(5)
N3	−0.2663(4)	0.18266(5)	0.7273(3)	0.0535(5)
O1	0.7156(3)	0.04690(4)	1.0016(2)	0.0506(4)
C1	0.6328(4)	0.00856(6)	0.6068(3)	0.0442(5)
H1A	0.729441	−0.018384	0.707226	0.053*
H1B	0.774324	0.023395	0.542616	0.053*
C2	0.5429(4)	0.04303(6)	0.7622(3)	0.0397(4)
C3	0.3589(4)	0.09646(6)	0.9171(3)	0.0386(4)
C4	0.1596(4)	0.13453(6)	0.9348(3)	0.0393(4)
C5	0.1986(4)	0.15872(7)	1.1536(4)	0.0537(6)
H5	0.352728	0.150724	1.297690	0.064*
C6	0.0056(5)	0.19465(7)	1.1536(4)	0.0575(6)
H6	0.028922	0.211711	1.297540	0.069*
C7	−0.2214(5)	0.20515(7)	0.9400(4)	0.0531(5)
H7	−0.351553	0.229392	0.943878	0.064*
C8	−0.0752(4)	0.14794(6)	0.7284(3)	0.0443(5)
H8	−0.102227	0.131856	0.580920	0.053*

Experimental details

H atoms were placed in calculated positions and treated as constrained on their parent atoms, with C—H = 0.93 or 0.97 Å and $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$.

***Corresponding author: Fei Liu,** College of Chemical Engineering, Eastern Liaoning University, No. 325, Wenhua Road, Yuanbao District, Dandong City, Liaoning Province, P.R. 118003, People's Republic of China, e-mail: berylliu8090@sina.com
Huang Fang, Fang Zhang and Qifan Chen: College of Chemical Engineering, Eastern Liaoning University, No. 325, Wenhua Road, Yuanbao District, Dandong City, Liaoning Province, P.R. 118003, People's Republic of China

Discussion

Many molecules containing a 1,2,4-oxadiazole moiety exhibit interesting pharmacological properties and biological activities [4–9]. Furthermore, the 1,2-bis-1,2,4-oxadiazol-5-yl)ethane core tecton is well known to construct coordination polymers [10]. As an ongoing part of our investigations, we report the preparation and structure of the title compound. The title compound is approximately planar and inversion symmetry is present (*cf*. the figure). The dihedral angle of C1–C1–C2–N1 is found to be 28.7(3)°. Each 3-(pyridin-3-yl)-1,2,4-oxadiazol-5-yl moiety is almost planar. In the crystal structure, molecules are liked through intermolecular forces.

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