

Pang Kairui, Xue Mei, Lan Guanchao, Li Yunlu and Wang Jianlong*

The crystal structure of imidazo[4,5-*e*][1,3]diazepine-4,6,8-triamine methanol solvate, $C_7H_{11}N_7O$

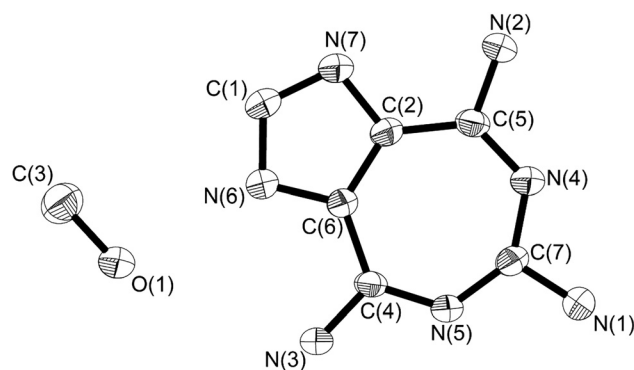


Table 1: Data collection and handling.

Crystal:	Block, colourless
Size:	0.11 × 0.08 × 0.05 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.11 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω -scans
$\theta_{\max}$, completeness:	27.5°, >99 %
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	8523, 2148, 0.106
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1081
$N(\text{param})_{\text{refined}}$:	155
Programs:	Bruker programs, ¹ SHELX, ^{2,3} OLEX2, ⁴

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Abstract

$C_7H_{11}N_7O$, monoclinic, $P2_1/c$ (no. 14), $a = 8.805(3)$ Å, $b = 7.483(3)$ Å, $c = 14.741(6)$ Å, $\beta = 105.719(6)^\circ$, $V = 934.9(6)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0646$, $wR_{\text{ref}}(F^2) = 0.1603$, $T = 296$ K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data. The list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

1 Source of material

2-Amino-4,5-dicyanoimidazole (133.0 mg, 1.0 mmol) was dissolved in 15 mL of ethanol. A methanol solution of guanidine

(64.9 mg, 1.1 mmol) was added to the mixture at room temperature, and the reaction was then heated to 80 °C and stirred for 10 h. After completion, the reaction mixture was cooled to room temperature, filtered, and recrystallized with methanol to afford the target compound 1 (117.1 mg, 61 % yield).

2 Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms. All the non-hydrogen atoms were refined anisotropically.

3 Discussion

Energetic materials, as energy materials critical to national strategic security, serve as the energy source for the propulsion, launch, and damage of weapon systems. With the continuous changes in the international landscape and the evolution of the times, the requirements for energetic materials are becoming increasingly stringent, particularly regarding safety performance to address factors during manufacturing, transportation, use, and storage. Nitrogen-containing fused ring skeletons, which consist of two or more nitrogen-containing rings fused together, are widely used in low-sensitivity high-energy energetic materials. Novel energetic materials based on nitrogen-containing fused ring skeletons have become a current research

*Corresponding author: Wang Jianlong, School of Chemistry and Chemical Engineering, North University of China, Taiyuan 030051, Shanxi Province, P.R. China, E-mail: wangjianlong@nuc.edu.cn

Pang Kairui, Xue Mei, Lan Guanchao and Li Yunlu, School of Chemistry and Chemical Engineering, North University of China, Taiyuan 030051, Shanxi Province, P.R. China. <https://orcid.org/0009-0002-5761-0929> (P. Kairui). <https://orcid.org/0000-0002-2210-5124> (X. Mei). <https://orcid.org/0000-0002-5292-7807> (L. Guanchao)

hotspot. However, at present, nitrogen-containing fused ring skeletons are primarily limited to three types: five-membered rings fused with five-membered rings, five-membered rings fused with six-membered rings, and six-membered rings fused with six-membered rings. The varieties of such fused ring skeletons are not only limited, but the scarcity of modification sites on these skeletons often necessary for attaching high-energy functional groups also restricts the development of new low-sensitivity high-energy energetic materials to some extent. Therefore, given the current lack of diversity in nitrogen-containing fused ring skeletons, developing novel nitrogen-containing fused ring skeletons is of great importance to the field of new energetic materials.^{5–10}

The crystal structure of the title compound features a unique penta-fused heptacyclic nitrogen-containing condensed ring structure, with its core skeleton comprising two heterocyclic systems: (1) a seven-membered heterocycle (formed by atoms C2, C4, C5, C6, C7, N4, and N5), in which the C4, C5, and C7 positions are modified with amino functional groups. The introduction of these amino groups significantly enhances the compound's reactivity and molecular diversity; (2) a five-membered heterocycle (containing atoms C1, C2, C6, N6, and N7), where the C1 position is substituted with a methyl group.

The dihedral angle between the plane formed by the seven-membered heterocycle and the plane formed by the five-membered heterocycle is 3.6°. The dihedral angle between the plane of the amino (N1) group and the plane of the seven-membered ring is 6.911°. The dihedral angle between the plane of the amino (N2) group and the plane of the seven-membered ring is 2.9°. The dihedral angle between the plane of the amino (N3) group and the plane of the seven-membered ring is 6.3°.

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