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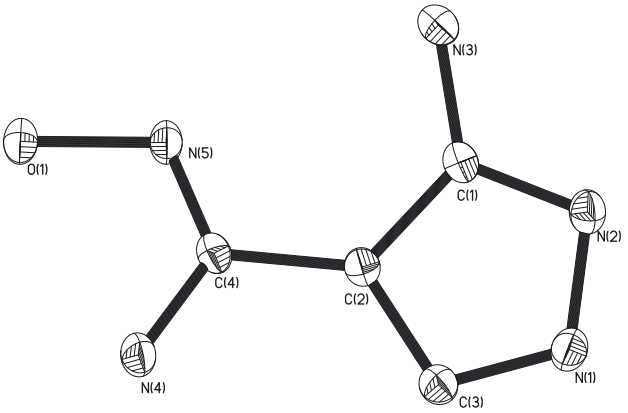
# The crystal structure of (*Z*)-5-amino-*N*′-hydroxy-1*H*-pyrazole-4-carboximidamide, $C_4H_7N_5O$

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**Abstract**

$C_4H_7N_5O$, monoclinic, $P2_1$ (no. 4), $a$ = 4.855(3) Å, $b$ = 9.026(5) Å, $c$ = 7.092(4) Å, $\beta$ = 103.267(7)°, $V$ = 302.5(3) Å$^3$, $Z$ = 2, $R_{gt}(F)$ = 0.0369, w$R_{ref}(F^2)$ = 0.0960, T = 296 K.

**CCDC no.:** 2375763

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.

## 1 Source of material

Add 0.01 mol 4-cyano-5-aminopyrazole and 20 mL methanol to the reactor. The temperature of the reactor was maintained at 298.15 K. Then add 1.35 g 50 % hydroxylamine aqueous solution to the reactor and the reaction lasts for 2 h. After the reaction is complete, the reaction solution is filtered. Remove the filtrate and retain the white solid precipitate. The white solid is dissolved in methanol and the solution is volatilized at room temperature to obtain clear colourless block shaped crystal. X-ray single crystal diffraction was performed on the crystal.

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**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Colourless block |
| Size: | 0.12 × 0.08 × 0.06 mm |
| Wavelength: | Mo *K*α radiation (0.71073 Å) |
| $\mu$: | 0.12 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 27.6°, >99 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 1,891, 1,218, 0.021 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\sigma(I_{obs})$, 1,154 |
| $N(param)_{refined}$: | 98 |
| Programs: | Olex2[1], SHELX[2,3], Bruker[4] |

## 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.

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

| Atom | *x* | *y* | *z* | $U_{iso}^*/U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.8029 (4) | 0.6763 (2) | 0.9073 (3) | 0.0355 (5) |
| H1 | 0.905 (7) | 0.752 (4) | 0.875 (2) | 0.053* |
| N1 | −0.1043 (5) | 0.3266 (3) | 0.4462 (3) | 0.0301 (5) |
| N2 | −0.0019 (5) | 0.4043 (3) | 0.3110 (3) | 0.0283 (5) |
| N3 | 0.3684 (5) | 0.5767 (3) | 0.3276 (3) | 0.0321 (5) |
| H3A | 0.322987 | 0.588313 | 0.203968 | 0.039* |
| H3B | 0.508591 | 0.625092 | 0.396301 | 0.039* |
| N4 | 0.5402 (5) | 0.4347 (3) | 0.9428 (3) | 0.0363 (6) |
| H4A | 0.666979 | 0.468677 | 1.038247 | 0.044* |
| H4B | 0.455321 | 0.352876 | 0.954953 | 0.044* |
| N5 | 0.5896 (5) | 0.6331 (3) | 0.7416 (3) | 0.0285 (5) |
| C1 | 0.2167 (5) | 0.4806 (3) | 0.4154 (3) | 0.0229 (5) |
| C2 | 0.2551 (5) | 0.4513 (3) | 0.6159 (3) | 0.0237 (5) |
| C3 | 0.0421 (5) | 0.3520 (3) | 0.6262 (4) | 0.0283 (6) |
| H3 | 0.007494 | 0.310557 | 0.738523 | 0.034* |
| C4 | 0.4749 (5) | 0.5096 (3) | 0.7747 (3) | 0.0243 (5) |
| H1A | −0.267 (8) | 0.274 (4) | 0.410 (5) | 0.043 (9)* |

## 3 Comment

Pyrazole compounds are research hotspots in the field of energetic materials in various countries.[5–9] The 4-cyano-5-aminopyrazole is an important imidazole compound that has been extensively studied.[10] The title compound was obtained by reacting 4-cyano-5-aminopyrazole and hydroxylamine aqueous solution. The title compound is an organic compound with high research value in the preparation of pyrazole energetic materials.

The asymmetric unit of the title compound is one (*Z*)-5-amino–*N*′-hydroxy-1*H*-pyrazole-4-carboximidamide molecule. The bond lengths and angles are in the expected ranges. The four atoms N4, C4, N5, O1 are in the same plane. The dihedral angle formed by pyrazole ring and plane of N4, C4, N5, O1 is 22.273°. Two intramolecular hydrogen bonds are formed in one molecule and the bond lengths of hydrogen bonds are 2.390 and 2.256 Å.

The title compound was obtained by reacting 4-cyano-5-aminopyrazole and hydroxylamine aqueous solution. During the reaction, hydroxylamine molecules are free in solution in the form $-NH_2$ and –OH. The –CN triple bond of 4-cyano-5-aminopyrazole becomes double bond, with the C atom connected to $-NH_2$ and the N atom connected to –OH, generating the title compound.

**Author contribution:** All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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**Conflict of interest statement:** The authors declare no conflicts of interest regarding this article.

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