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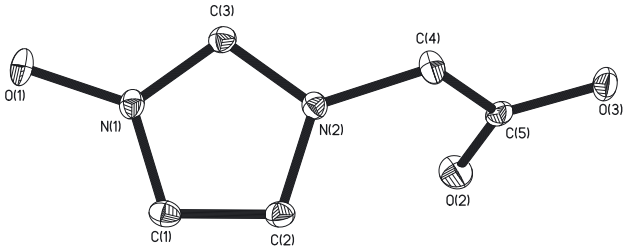
The crystal structure of 1-(carboxymethyl)-1*H*-imidazole 3-oxide



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Abstract

$C_5H_6O_3N_2$, monoclinic, $P2_1/c$ (no. 14), a = 11.3451(10) Å, b = 4.9505(5) Å, c = 10.3200(8) Å, β = 99.220(3)°, V = 572.12(9) Å^3, Z = 4, $R_{gt}(F)$ = 0.0429, $wR_{ref}(F^2)$ = 0.1031, T = 170 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.

1 Source of material

Formaldehyde, glyoxal, glycine, and hydroxylamine were added to the reactor. The temperature of the reactor was 278.15 K. Turn on the mixer at a speed of 500 r/min. The raw material underwent a condensation reaction in the reactor. After the reaction, the white solid was obtained. Dissolve the white solid in deionized water and pour it into an evaporating dish. Place the evaporating dish at room temperature and evaporate deionized water to obtain colorless block crystals.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.08 × 0.07 × 0.04 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.14 mm^{-1}
Diffractometer, scan mode:	D8 VENTURE, φ and ω
θ_{max}, completeness:	26.4°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6091, 1175, 0.082
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 895
$N(param)_{refined}$:	99
Programs:	Olex2 [1], SHELX [2, 3], Bruker [4]

2 Experimental details

Hydrogen atom was placed in their geometrically idealized positions and constrained to ride on their parent atoms.

3 Comment

Imidazole compounds have always been a hot research topic in the field of organic chemistry [5–8]. The title compound is obtained by condensation reaction of formaldehyde, glyoxal, glycine, and hydroxylamine. The title compound is an imidazole oxide and has high research value as an organic intermediate.

The asymmetric unit of the title compound is 1-(carboxymethyl)-1H-imidazole 3-oxide molecule. The bond lengths and angles are in the expected ranges. All non-hydrogen atoms of the molecule are on two planes. The seven atoms of O1, C3, N1, C1, C2, N2 and C4 are on the first plane. The four atoms of C4, C5, O2 and O3 are on the second plane. The dihedral angle of two planes is 67.230°. On the first glance, C3, N1, C1, C2, and N2 form a five membered ring structure. This five membered ring is an imidazole structure, which is the same as the imidazole structure reported in the literature [9, 10].

Both O1 and O3 atoms are connected to a hydrogen atom. The two molecules of the title compound are connected by hydrogen bonds around two inversion centers (O1···O1′; O3···O3″). According to the above connection pattern, the title compound molecule forms a chain like compound.

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.64993 (18)	0.5567 (4)	0.92669 (18)	0.0199 (4)
H1A	0.623048	0.436429	0.987468	0.024*
C2	0.75250 (18)	0.5384 (4)	0.87647 (17)	0.0192 (4)
H2	0.811914	0.402670	0.895750	0.023*
C3	0.65573 (16)	0.9004 (4)	0.79112 (17)	0.0173 (4)
H3A	0.634855	1.059429	0.741177	0.021*
C4	0.85311 (17)	0.8193 (4)	0.72301 (18)	0.0213 (5)
H4A	0.927344	0.833476	0.787741	0.026*
H4B	0.837683	0.998538	0.681154	0.026*
C5	0.87265 (17)	0.6159 (4)	0.61864 (17)	0.0183 (4)
N1	0.59215 (13)	0.7838 (3)	0.87250 (14)	0.0179 (4)
N2	0.75488 (13)	0.7530 (3)	0.79216 (14)	0.0168 (4)
O1	0.48387 (12)	0.8741 (3)	0.89628 (13)	0.0236 (4)
H1[a]	0.494 (5)	0.974 (9)	0.965 (3)	0.028 (13)*
O2	0.80649 (13)	0.4227 (3)	0.59011 (13)	0.0265 (4)
O3	0.96733 (12)	0.6759 (3)	0.56970 (13)	0.0241 (4)
H3[a]	0.996 (5)	0.550 (9)	0.524 (5)	0.034 (13)*

[a]Occupancy: 0.5.

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

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