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The crystal structure of 1-(2-carboxyethyl)-1*H*-imidazole 3-oxide

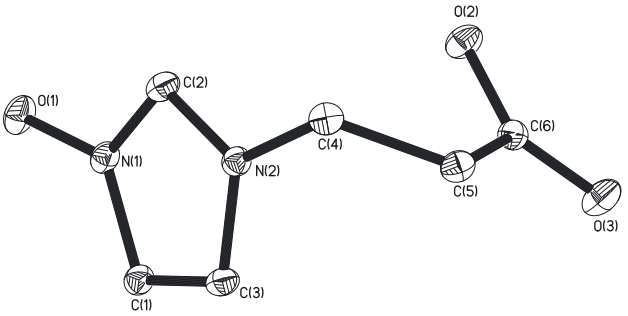

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.15 × 0.08 × 0.05 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.13 mm^{-1}
Diffractometer, scan mode:	D8 VENTURE, φ and ω
θ_{max}, completeness:	27.5°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5847, 1519, 0.053
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1230
$N(param)_{refined}$:	101
Programs:	Olex2,[1] SHELX,[2,3] Bruker[4]

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Abstract

$C_6H_8N_2O_3$, monoclinic, $P2_1/n$ (no. 14) a = 5.2014(4) Å, b = 13.4511(9) Å, c = 9.6808(6) Å, β = 97.867(3)°, V = 670.94(8) Å^3, Z = 4, $R_{gt}(F)$ = 0.0451, w$R_{ref}(F^2)$ = 0.1308, 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, alanine, and hydroxylamine were added to the reactor. The temperature of the reactor is maintained at 298 K. Turn on the mixer at a speed of 500 r/min. The reaction is for 2 h. The raw material underwent a condensation reaction in the reactor. After the reaction, the white solid was obtained. The reaction solution is filtered to remove the filtrate and retain the white solid. 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. X-ray single crystal diffraction was performed on the crystal.

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 Comment

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

The asymmetric unit of the title compound is one 1-(2-carboxyethyl)-1H-imidazole 3-oxide molecule. The bond lengths and angles are in the expected ranges. The six atoms of O1, N1, C1, C3, N2, C2 are in the same plane. The four atoms of C5, C6, O2, O3 are also in the

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5068 (4)	0.28523 (15)	0.67864 (19)	0.0193 (4)
H1A	0.656390	0.244046	0.693651	0.023*
C2	0.1669 (4)	0.36746 (16)	0.57164 (19)	0.0200 (4)
H2	0.039872	0.393095	0.500747	0.024*
C3	0.3902 (4)	0.33332 (16)	0.77700 (19)	0.0198 (4)
H3	0.443633	0.332063	0.874832	0.024*
C4	0.0131 (4)	0.45332 (16)	0.77337 (19)	0.0206 (4)
H4A	−0.096928	0.415220	0.830283	0.025*
H4B	−0.102720	0.488291	0.699315	0.025*
C5	0.1705 (4)	0.52913 (16)	0.86489 (19)	0.0203 (4)
H5A	0.268562	0.493659	0.944929	0.024*
H5B	0.048416	0.574924	0.902702	0.024*
C6	0.3614 (4)	0.59113 (15)	0.79537 (19)	0.0182 (4)
N1	0.3632 (3)	0.30865 (13)	0.55324 (15)	0.0181 (4)
N2	0.1807 (3)	0.38411 (12)	0.70880 (16)	0.0176 (4)
O1	0.4114 (3)	0.27341 (11)	0.42680 (13)	0.0239 (4)
H1	0.508055	0.313458	0.391672	0.036*
O2	0.3189 (3)	0.59739 (11)	0.66139 (13)	0.0234 (4)
O3	0.5400 (3)	0.63287 (12)	0.86967 (14)	0.0277 (4)

same plane. The dihedral angle of two planes is 73.3°. On the first plane, N1, C1, C3, N2 and C2 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] C4 atom is not on the two planes mentioned above. The line to surface angle of C4–N2 and plane of O1, N1, C1, C3, N2, C2 is 4.75°. The line to surface angle of C4–C5 and plane of C5, C6, O2, O3 is 18.0°.

The title compound is an imidazole oxide, and similar structures have been published.[11,12] The structure of the title compound is similar to that of these substances. Imidazole structures were generated through condensation reactions. There are two N atoms in the imidazole structure, one of which is connected to an O atom, and the other N atom is connected to a long chain structure with carboxylic acid. The difference between them is the number of C atoms in the long chain structure.

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