

Crystal structure of 2-amino-1,3,4-oxadiazole, $C_2H_3N_3O$ (NH_2)

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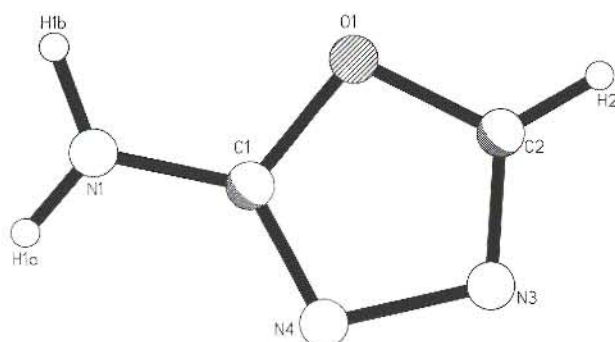


Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.85 × 0.8 × 0.6 mm
Wavelength:	Mo K_{α} radiation (0.71073 Å)
μ :	1.00 cm ⁻¹
Diffractometer, scan mode:	Siemens P4, ω
$2\theta_{\max}$:	55°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	949, 790
Criterion for F_{obs} , $N(hkl)_{\text{gt}}$:	$F_{\text{obs}} > 3 \sigma(F_{\text{obs}})$, 771
$N(\text{param})_{\text{refined}}$:	63
Program:	SHELXTL-plus [3]

Abstract

$C_2H_3N_3O$, monoclinic, $P12_1/n1$ (No. 14), $a = 4.426(3)$ Å, $b = 8.763(3)$ Å, $c = 9.079(3)$ Å, $\beta = 97.63(2)^\circ$, $V = 349.0$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.053$, $wR(F) = 0.060$, $T = 293$ K.

Source of material

The title compound was synthesized by reaction of 1-formylthiosemicarbazide with lead(II)oxide in ethanol [1] or by reaction of formic acid hydrazide with bromocyanogen [2].

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(1A)	4e	0.738(5)	0.141(3)	0.057(2)	0.061(6)
H(1B)	4e	0.459(5)	0.180(3)	-0.061(3)	0.063(6)
H(2)	4e	0.1242(4)	0.5823(2)	0.1856(2)	0.08

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	4e	0.5785(4)	0.1981(2)	0.0297(2)	0.054(1)	0.0486(9)	0.0369(9)	0.0109(7)	-0.0092(7)	-0.0076(7)
C(1)	4e	0.5118(3)	0.3094(2)	0.1197(2)	0.0337(8)	0.0384(9)	0.0295(8)	-0.0045(6)	-0.0024(6)	0.0049(6)
O(1)	4e	0.2729(2)	0.4016(1)	0.0704(1)	0.0431(7)	0.0447(8)	0.0295(7)	0.0044(5)	-0.0045(5)	-0.0022(5)
C(2)	4e	0.2709(4)	0.5016(2)	0.1853(2)	0.049(1)	0.044(1)	0.036(1)	-0.0016(7)	0.0034(7)	-0.0051(8)
N(3)	4e	0.4813(3)	0.4757(2)	0.2927(2)	0.0510(9)	0.0473(9)	0.0339(8)	-0.0042(6)	0.0004(6)	-0.0046(7)
N(4)	4e	0.6430(3)	0.3466(2)	0.2512(1)	0.0516(9)	0.0430(9)	0.0283(8)	-0.0010(6)	-0.0061(6)	-0.0001(6)

References

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