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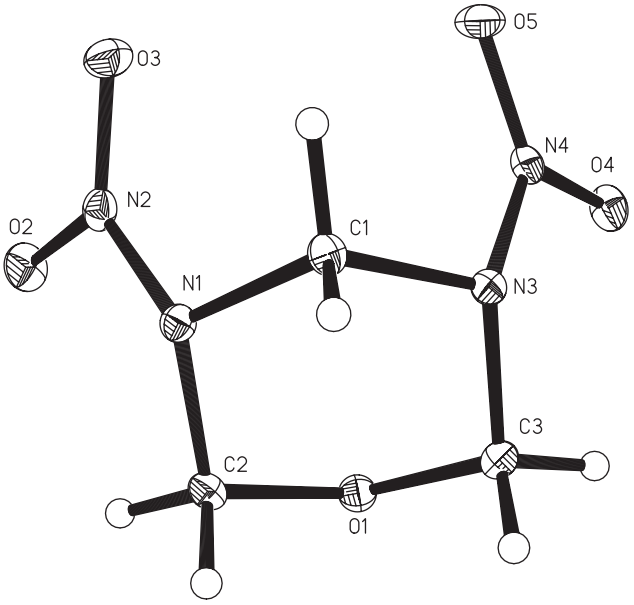
The crystal structure of 3,5-dinitro-1,3,5-oxadiazinane, $C_3H_6N_4O_5$



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Abstract

$C_3H_6N_4O_5$, monoclinic, $P2_1/n$ (no. 14), $a = 5.8128(13)$ Å, $b = 17.2389(14)$ Å, $c = 7.1072(6)$ Å, $\beta = 112.056(16)°$, $V = 660.06(16)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0330$, $wR_{ref}(F^2) = 0.0752$, $T = 103.0$ K.

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The crystal structure is shown in the figure. Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound, $C_3H_6N_4O_5$, was prepared from hexamine by nitration. It was recrystallized from acetone solution at room temperature to give colorless crystals suitable for single-crystal X-ray diffraction.

Table 1: Data collection and handling.

Crystal:	Colorless, block, size 0.25×0.30×0.35 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	1.69 cm^{-1}
Diffractometer, scan mode:	Xcalibur, Eos, Gemini, ω scans
$2\theta_{max}$:	51.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2543, 1292
$N(param)_{refined}$:	109
Programs:	CrysAlis [1], SHELX [2], OLEX2 [3]

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

Atom	Site	x	y	z	U_{iso}
H(1A)	4*e*	0.4880	0.2284	0.3376	0.018
H(1B)	4*e*	0.7744	0.2202	0.3902	0.018
H(2A)	4*e*	0.9952	0.1153	0.6820	0.020
H(2B)	4*e*	0.8248	0.0814	0.7888	0.020
H(3A)	4*e*	0.7108	0.0207	0.2311	0.023
H(3B)	4*e*	0.9213	0.0805	0.3434	0.023

Experimental details

H atoms were positioned geometrically with C—H = 0.97 , and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2$ times $U_{eq}(C)$.

Discussion

3,5-dinitro-1,3,5-oxadiazinane is obtained as a by-product in the synthesis of RDX (1,3,5-trinitro-1,3,5-triazinane) from hexamine by nitration. As part of our search for nitrlysis mechanism of hexamine, the title compound was separated and its structure was characterized. As shown in the figure, the oxadriazine ring adopts a chair conformation two nitro groups stand on the same side of the triazine ring.

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Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(5)	4*e*	0.1737(2)	0.15476(6)	0.1268(2)	0.0171(6)	0.0209(6)	0.0266(6)	0.0058(5)	0.0023(5)	−0.0012(5)
O(1)	4*e*	0.7543(2)	0.03820(6)	0.5165(2)	0.0187(6)	0.0156(6)	0.0170(5)	0.0019(5)	0.0060(4)	0.0008(4)
O(4)	4*e*	0.2911(2)	0.03919(6)	0.0812(2)	0.0291(7)	0.0136(6)	0.0181(6)	−0.0036(5)	0.0067(5)	−0.0028(4)
O(3)	4*e*	0.2843(2)	0.21255(7)	0.5482(2)	0.0177(6)	0.0255(7)	0.0275(6)	0.0046(5)	0.0087(5)	0.0002(5)
N(3)	4*e*	0.5807(2)	0.12716(7)	0.2461(2)	0.0131(6)	0.0182(7)	0.0133(6)	0.0007(5)	0.0039(5)	−0.0016(5)
O(2)	4*e*	0.4584(2)	0.12849(7)	0.7875(2)	0.0269(7)	0.0323(7)	0.0187(6)	−0.0018(5)	0.0137(5)	0.0048(5)
N(2)	4*e*	0.4534(2)	0.16813(8)	0.6428(2)	0.0172(7)	0.0183(7)	0.0166(7)	−0.0037(6)	0.0069(6)	−0.0049(5)
N(1)	4*e*	0.6610(2)	0.16624(7)	0.5909(2)	0.0145(6)	0.0162(7)	0.0136(6)	−0.0003(5)	0.0068(5)	0.0006(5)
N(4)	4*e*	0.3322(2)	0.10517(8)	0.1487(2)	0.0180(7)	0.0162(7)	0.0115(6)	−0.0006(6)	0.0047(5)	0.0014(5)
C(1)	4*e*	0.6270(3)	0.19269(9)	0.3860(2)	0.0168(8)	0.0154(8)	0.0142(7)	−0.0013(6)	0.0062(6)	0.0008(6)
C(2)	4*e*	0.8269(3)	0.09954(9)	0.6603(2)	0.0143(8)	0.0187(8)	0.0148(7)	−0.0008(6)	0.0031(6)	0.0000(6)
C(3)	4*e*	0.7556(3)	0.06351(9)	0.3265(2)	0.0193(8)	0.0228(9)	0.0174(8)	0.0055(7)	0.0084(7)	0.0005(6)

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