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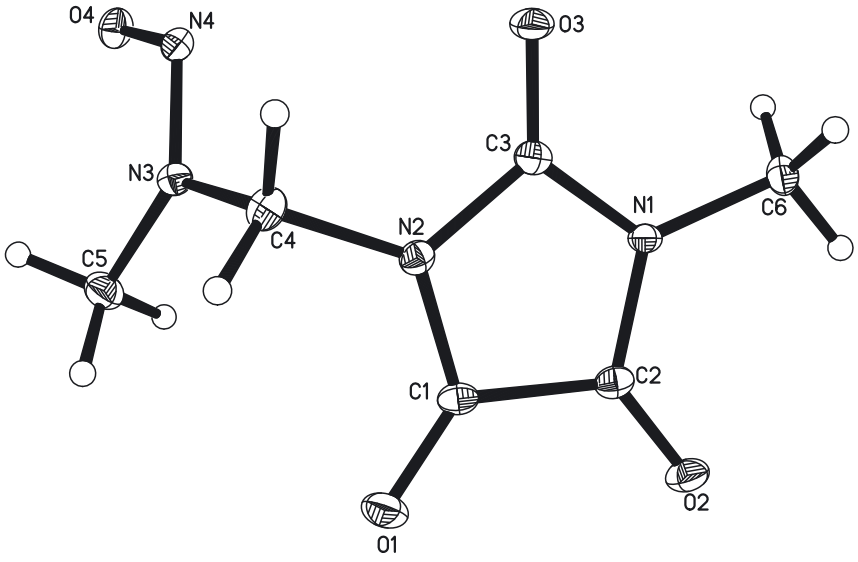
The crystal structure of 1-methyl-3-(N-methylnitrous amide–N-methylene) imidazolidine-2,4,5-trione



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Abstract

$C_6H_8O_4N_4$, orthorhombic, $Pna2_1$ (no. 33), a = 6.5487(4) Å, b = 17.5223(9) Å, c = 7.5728(4) Å, V = 868.97(8) Å^3, Z = 4, R_{gt}(F) = 0.0740, wR_{ref} (F^2) = 0.0761, T = 106.0 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.

Table 1: Data collection and handling.

Crystal:	block
Size:	0.40 × 0.35 × 0.15 mm
Wavelength:	MoKα radiation (0.71073 Å)
μ:	0.13 mm^{-1}
Diffractometer, scan mode:	Xcalibur, Eos, Gemini, φ and ω scans
θ_{max}, completeness:	26.0°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	3112, 1612, 0.026
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1,530
$N(param)_{refined}$:	129
Programs:	Rigaku,[1] Olex2,[2] SHELX[3,4]

1 Source of material

An amount of 0.2 g of 1-methyl-3-(N-methylnitrous amide–N-methylene)imidazolidine-2,4,5-trione was added to 5 ml of methanol and evaporated at room temperature to give colorless block crystals.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4777 (3)	0.98274 (10)	0.2486 (3)	0.0284 (5)
O2	0.1086 (3)	0.99297 (10)	0.4813 (3)	0.0249 (5)
O3	0.5304 (3)	0.80631 (9)	0.6911 (2)	0.0263 (5)
O4	0.7007 (3)	0.67930 (10)	0.2076 (2)	0.0223 (5)
N1	0.2743 (3)	0.89228 (12)	0.6179 (3)	0.0161 (5)
N2	0.5581 (3)	0.88764 (12)	0.4497 (3)	0.0166 (5)
N3	0.7308 (3)	0.80105 (12)	0.2525 (3)	0.0167 (5)
N4	0.7354 (3)	0.73085 (12)	0.3168 (3)	0.0188 (5)
C1	0.4395 (4)	0.94426 (14)	0.3765 (3)	0.0189 (6)
C2	0.2483 (4)	0.94871 (15)	0.4952 (4)	0.0182 (6)
C3	0.4619 (4)	0.85584 (13)	0.5981 (3)	0.0181 (6)
C4	0.7543 (4)	0.86032 (16)	0.3840 (4)	0.0209 (6)
H4A	0.828936	0.902718	0.332792	0.025*
H4B	0.833870	0.840649	0.481958	0.025*
C5	0.6891 (5)	0.81782 (16)	0.0680 (4)	0.0250 (7)
H5A	0.755578	0.780663	−0.005253	0.037*
H5B	0.739611	0.867779	0.039830	0.037*
H5C	0.544441	0.816083	0.047669	0.037*
C6	0.1395 (5)	0.87887 (15)	0.7695 (4)	0.0249 (7)
H6A	0.095577	0.826603	0.769584	0.037*
H6B	0.022570	0.911733	0.761351	0.037*
H6C	0.212121	0.889513	0.876860	0.037*

2 Experimental details

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

3 Discussion

1–Methyl-2,4,5-trinitroimidazole is an energetic compound with good performance.[5,6] 1–Methyl-2,4,5-trinitroimidazole is obtained by nitration of 1-methyl-2,4,5-triiodoimidazole with a mixture of HNO_3 and H_2SO_4.[7–10] The title compound was obtained by nitration of 1-methyl-2,4,5-triiodoimidazole with a mixture of HNO_3 and H_2SO_4 in DMF solution.

The crystal structure of the title compound was analyzed and refined by Shelxl program.[1–4] As shown in the figure, the asymmetric unit contains one title molecule. The bond lengths and angles within these moieties are in the expected ranges.[11,12] The imidazole rings are planar, the carbon atoms of the methyl group (N1) and the methylene group (N2), the oxygen atom of the carbonyl group are nearly coplanar with the imidazole ring. However, all other atoms are twisted out of the imidazole ring.

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