

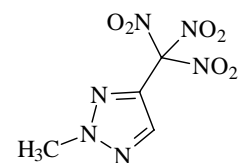
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ED

C₄H₄N₆O₆

2-Methyl-4-trinitromethyl-2*H*-1,2,3-triazole

C₁

r_a	\AA^a	θ_a	deg^a
N=C	1.358(5)	N–N–N	117.6 ^{b)}
N–N	1.314(3)	N–N=C	103.0(3)
N–C(CH ₃)	1.450 ^{b)}	C–C–C	130.0(9)
C(ring)–C	1.444(7)	C–C–N	109.6(4)
C(ring)–C(ring) ^{c)}	1.385(12)	C–N=O	114.9(2)
C–N	1.528(2)	H–C–H	102.4 ^{b)}
N=O	1.201(2)	$\phi(\text{C}(\text{ring})\text{--C})^d)^e)$	33.0(20)
C–H	1.105 ^{b)}	$\phi(\text{C--N})^d)^f)$	35.4(40)
		$\phi(\text{C--N})^d)^g)$	68.7(30)
		$\phi(\text{C--N})^d)^h)$	43.4(30)



Local C_{2v} symmetry of the triazole ring and threefold symmetry of the N₃C fragment with no tilt were assumed.
The nozzle temperature was 110(10) °C.

^{a)} Estimated standard errors.

^{b)} Assumed.

^{c)} Dependent parameter.

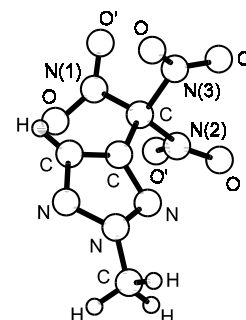
^{d)} The positive direction of the torsional angles ϕ corresponds to a clockwise rotation about the (C(ring)–C) and (C–N) bonds from staggered conformation.

^{e)} Torsional angle C–C–C–N(1).

^{f)} Torsional angle C–C–N(1)–O.

^{g)} Torsional angle C–C–N(2)–O.

^{h)} Torsional angle C–C–N(3)–O.



Belyakov, A.V., Levit, P.B., Tselinskii, I.V., Shlyapochnikov, V.A., Ladyzhnikova, T.D., Altukhov, K.V., Manuel, D.V.: J. Mol. Struct. **265** (1992) 337.