

1794
MW

C₄H₉NO₂

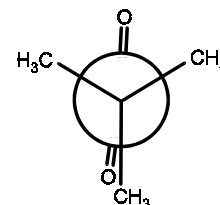
2-Methyl-2-nitropropane

C_s^{a)}
O₂N-C(CH₃)₃

r_0	Å ^{a)}
C-N	1.53(2)

^{a)} Effective symmetry is higher.

Langridge-Smith, P.R.R., Stevens, R., Cox, A.P.: J. Chem. Soc., Faraday Trans. II **76** (1980) 330.



ED

r_g	Å ^{a)}	θ_g	deg ^{a)}
N=O	1.240(2)	O=N=O	122.2(6)
C-N, C-C (mean) ^{b)}	1.533(15)	C-C-C	110.9(11)
C-H	1.102(5)	H-C-H	107.9(9)

The NO₂, CH₃ and C(CH₃)₃ groups were assumed to have C_{2v}, C_{3v} and C_{3v} symmetry, respectively. The experimental data do not contradict the model of free internal rotation of the NO₂ group about the C-N bond.

The nozzle temperature was 30(5) °C.

^{a)} Three times the estimated standard errors without explicit statement of the systematic error.

^{b)} It was impossible to separate the C-N and C-C bond lengths in the least-squares analysis.

Shishkov, I.F., Sadova, N.I., Vilkov, L.V., Pankrushev, Yu.A.: Zh. Strukt. Khim. **24** No.2 (1983) 25; Russ. J. Struct. Chem. (Engl. Transl.) **24** (1983) 189.