

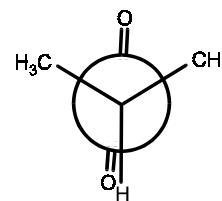
1332
MW

C₃H₇NO₂

2-Nitropropane

C_s
O₂N-CH(CH₃)₂

r_0	Å	θ_0	deg ^{a)}
N=O	1.218(30)	C-C-C	112.7 ^{b)}
C-N	1.508(36)	N-C-C	108.9(34)
C-C	1.533(12)	C-C-H	110.8 ^{b)}
C-H	1.092 ^{b)}	C-N=O	116.8(30)



One N=O bond is eclipsed with respect to the C-H bond, see figure.

^{a)} Uncertainties are about twice those of the original paper.

^{b)} Assumed.

Durig, J.R., Smooter Smith, J.A., Li, Y.S., Wasacz, F.M.: J. Mol. Struct. **99** (1983) 45.

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r_g	Å ^{a)}	θ_g	deg ^{a)}
N=O	1.226(2)	O=N=O	125.4(3)
C-N, C-C (mean) ^{b)}	1.518(10)	C-C-C	113.5(17)
C-H	1.092(4)	N-C-C	109.2(9)
		H-C-H	106.9(15)
		N-C-H	106.4(61)

The NO₂ and CH₃ groups were assumed to have C_{2v} and C_{3v} symmetry, respectively.

The nozzle temperature was 30(5) °C.

^{a)} Three times the estimated standard errors.

^{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.