

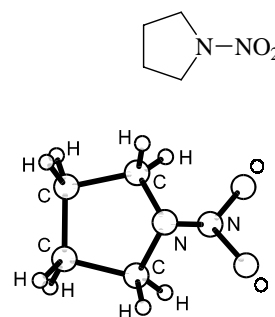
1731
ED

C₄H₈N₂O₂

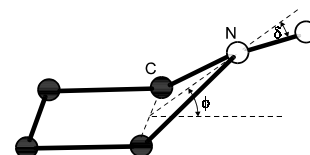
***N*-Nitropyrrolidine**

essentially C_s

r_g	Å ^{a)}	θ_α	deg ^{a)}
C–N	1.477(8)	C–C–N	96.6(4)
C–C	1.534(5)	C–N–C	110.3(14)
N–N	1.363(4)	C–N–N	116.0(11)
N=O	1.225(2)	O=N=O	126.3(19)
C–H	1.098(8)	H–C–H	108.6(68)
		$\tau(\text{NN})$ ^{b)}	16.8(16)
		ϕ ^{c)}	42.2(25)
		δ ^{d)}	39.9(50)
		γ ^{e)}	342.3(50)



The conformation of the five-membered ring is an envelope of C_s symmetry. The NO₂ group is located in the equatorial position. The nozzle was at different temperatures, 68 and 152 °C; both measurements were used to derive the listed structure.



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

^{b)} Torsional angle about the N–N bond. The value 0° corresponds to a position of the NO₂ groups such that the line segments C–C and O–O for C₂N–NO₂ will lie in a single plane.

^{c)} Angle between the CNC and CCCC planes. Dependent parameter.

^{d)} Angle between the N–N bond and the CNC plane. Dependent parameter.

^{e)} The sum of the bond angles at the amine N atom.

Shishkov, I.F., Vilkov, L.V., Pyatakov, N.F.: Zh. Strukt. Khim. **33** No.1 (1992) 46; Russ. J. Struct. Chem. **33** (1992) 38.

Shishkov, I.F., Vilkov, L.V., Kolonits, M., Rozsondai, B.: Struct. Chem. **2** (1991) 57.