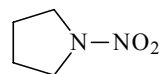


558 **C₄H₈N₂O₂**ED, *ab initio*
calculations**1-Nitropyrrolidine***N*-Nitropyrrolidine**C₁**

r_g	Å ^{a)}	θ_a	deg ^{a)}
N(1)–C(2) ^{b)}	1.481(18)	H–C–H	111.0(28)
C(2)–C(3) ^{b)}	1.524(18)	O=N=O	124.6(12)
C(3)–C(4) ^{b)}	1.537(18)	C(5)–N(1)–C(2)	112.5(22)
C(4)–C(5) ^{b)}	1.537(18)	N(1)–C(2)–C(3)	102.6(18)
C(5)–N(1) ^{b)}	1.489(18)	C(2)–C(3)–C(4)	102.6(20)
N–N	1.376(5)	C(3)–C(4)–C(5)	105.2(20)
N=O	1.230(3)	C(4)–C(5)–N(1)	102.6(10)
C–H	1.111(5)	C–N–N	117.1(12)
		τ_1 ^{c)}	324.8(22)
		τ_2 ^{d)}	37.7(18)
		τ_3 ^{e)}	335.4(10)
		τ_4 ^{f)}	2.1(8)
		τ_5 ^{g)}	21.1(22)
		q_0 ^{h)}	10.8(6)
		f^i	76.0(16)
		φ^j	35.1(22)
		$\tau(\text{NO}_2)$ ^{k)}	0.2(34)

Experimental intensities obtained in [1] were reanalyzed. According to ED data and results of HF/6-311++G** calculations, the molecule has C(3)-envelope conformation of the pyrrolidine ring (E³ or its enantiomeric E⁴ form). This conformation differs from N(1)-envelope conformation (E¹) reported in the previous ED investigation [1] (the C(3)-envelope form was not tested in this study). The barrier to inversion at the ring nitrogen, *i.e.*, the energy difference between the transition state B and the stable conformation A, was estimated to be 3.7 kJ mol^{−1} by the MP2/6-311++G** method. Each CH₂ group was assumed to have local C_{2v} symmetry with one of the symmetry planes passing through the H–C–H atoms and the other being formed by the carbon atom of the CH₂ group and two adjacent atoms in the ring. The NNO₂ moiety was assumed to be planar. The nozzle was at different temperatures, 68 and 152 °C; both measurements were used to derive the listed structure at 110 °C.

^{a)} Twice the estimated standard errors including a systematic error.

^{b)} Differences in the C–C and C–N bonds were assumed at the values from MP2/6-311++G** calculations.

^{c)} N(1)–C(2)–C(3)–C(4) torsional angle.

^{d)} C(2)–C(3)–C(4)–C(5) torsional angle.

^{e)} C(3)–C(4)–C(5)–N(1) torsional angle.

^{f)} C(4)–C(5)–N(1)–C(2) torsional angle.

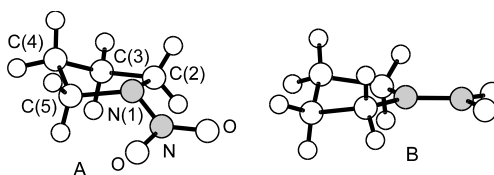
^{g)} C(5)–N(1)–C(2)–C(3) torsional angle.

^{h)} Puckering amplitude.

ⁱ⁾ Pseudorotation phase angle.

^{j)} Deviation of the N–N bond from the bisector of the C–N–C angle in the direction opposite to that of the C(3) out-of-plane atom in the ring.

^{k)} Torsional angle of the NO₂ group; 90 ° when one of the N=O bonds is eclipsed with respect to the bisector of the C–N–C angle.



Borisenko, K.B., Samdal, S., Shishkov, I.F., Vilkov, L.V.: Acta Chem. Scand. **52** (1998) 312.

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

Replaces [II/25C \(3, 1731\)](#)