

**1792 C<sub>4</sub>H<sub>9</sub>N**ED, *ab initio* calculations

(HF/4-21 (for C, N),

HF/21 (for H))

**Pyrrolidine****C<sub>s</sub>**

$r_a$	$\text{\AA}^a$	$\theta_a$	deg <sup>a)</sup>
C–N	1.469(10)	C–N–C	105.2(35)
C–C	1.543(8)	H–C–H	106.0(18)
C–H	1.090(4)	C–N–H	107.0 <sup>b)</sup>
N–H	1.020 <sup>b)</sup>	N–C–C	104.6 <sup>c)</sup>
		C–C–C	104.9 <sup>c)</sup>
		$\varphi$ <sup>d)</sup>	39.0(14)

The ED and *ab initio* calculation agree with respect to the most stable conformation shown in the figure. The calculation of the energy profile for pseudorotation results in a second energy minimum for the envelope conformer with the equatorial position of the amino H. The energy difference between these two conformers is predicted to be about 1 kcal mol<sup>−1</sup> and the barrier to pseudorotation to be 1.66 kcal mol<sup>−1</sup>.

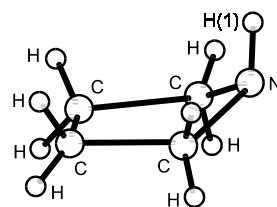
The nozzle temperature was 20 °C.

<sup>a)</sup> Three times the estimated standard errors.

<sup>b)</sup> Assumed.

<sup>c)</sup> Dependent parameter.

<sup>d)</sup> Flap angle of the CNC plane.



Pfafferott, G., Oberhammer, H., Boggs, J.E., Caminati, W.: J. Am. Chem. Soc. **107** (1985) 2305.

**MW**

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
H(1)	1.3439	0.1505	1.2122

Caminati, W., Oberhammer, H., Pafferott, G., Filgueira, R.R., Gomez, C.H.: J. Mol. Spectrosc. **106** (1984) 217.