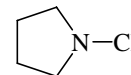


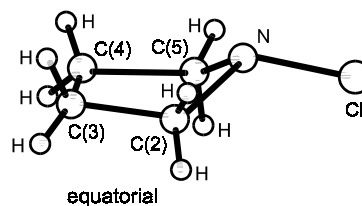
ED, *ab initio* calculations

(HF/4-21, etc.)

$r_a$	$\text{\AA}^a$		$\theta_a$	$\text{deg}^a$	
	axial	equatorial		axial	equatorial
C(2)–N	1.480	1.476(5)	C–N–C	106.4	108.0(8)
C(2)–C(3)	1.540	1.535(3)	C(2)–N–Cl	108.0	110.5(7)
C(3)–C(4)	1.547	1.553(3)	H–C–H	105.3	105.3(22)
N–Cl	1.759	1.736(3)	wag (CH <sub>2</sub> ) <sup>b</sup>	–4.5 °	–1.6 °
C–H	1.086	1.086(4)	rock (CH <sub>2</sub> ) <sup>b</sup>	4.4 °	0.5 °
			$\varphi^d$	35.7	44.7(13)



The molecule exists as a mixture of the equatorial and axial conformers in a ratio of about 4:1. The differences in the parameters between the two conformers were constrained to *ab initio* values. The nozzle temperature was 35 °C.

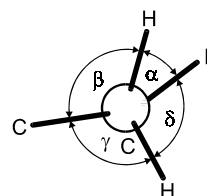


<sup>a</sup>) Three times the estimated standard errors.

<sup>b</sup>)  $\text{wag} = (1/2)[(\alpha + \delta) - (\beta + \gamma)]$ ,  
 $\text{rock} = (1/2)[(\alpha + \beta) - (\gamma + \delta)]$ . See figure for definitions. The differences from those for C(3) methylene group were constrained to *ab initio* values.

<sup>c</sup>) Fixed at the *ab initio* values.

<sup>d</sup>) Dihedral angle between the CNC and CCCC planes.



Pfafferott, G., Oberhammer, H., Boggs, J.E.: J. Am. Chem. Soc. **107** (1985) 2309.