

**1240 C<sub>3</sub>H<sub>6</sub>ClNO**ED, *ab initio*calculations (MP2/6-31G\*\*) **C<sub>1</sub>****Dimethylcarbamic chloride**

Dimethylcarbamoyl chloride

**C<sub>1</sub>**  
Cl(O)C–N(CH<sub>3</sub>)<sub>2</sub>

$r_g$	Å <sup>a)</sup>
C=O	1.202(3)
C(4)–N	1.365(3)
C(2)–N <sup>b)</sup>	1.461(6)
C(3)–N <sup>b)</sup>	1.464(6)
C–Cl	1.789(4)
C–H	1.117(3)

$\theta_a$	deg <sup>a)</sup>
N–C=O	126.5(2)
N–C–Cl	113.9(3)
C(2)–N–C(4)	116.0(4)
C(3)–N–C(4) <sup>b)</sup>	124.8(4)
C(2)–N–C(3) <sup>b)</sup>	116.2(3)
N–C–H	110.8(3)
C(2)–N–C(4)=O <sup>c)</sup>	13.0(25)
C(3)–N–C(4)=O <sup>b) c)</sup>	172.5(36)
C(4)–N–C(2)–H(1) <sup>d)</sup>	–11.7(40)
C(4)–N–C(3)–H(4) <sup>b) d)</sup>	45.3(24)

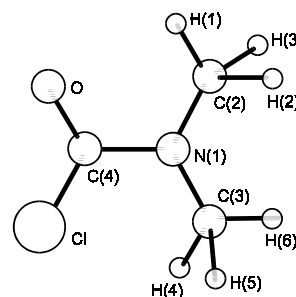
The methyl groups were assumed to have local C<sub>3v</sub> symmetry. The bond configuration around the N atom is essentially planar. Differences in similar parameters were constrained to *ab initio* values. The nozzle was at about 33 °C.

<sup>a)</sup> Estimated total errors.

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

<sup>c)</sup> Torsion angle is 0° when the C–N and C–O bonds are eclipsed.

<sup>d)</sup> Torsion angle is 0° when the C–N and C–H bonds are eclipsed.



Schultz, G., Hargittai, I.: J. Phys. Chem. **99** (1995) 11412.