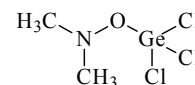
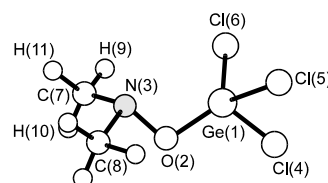


**298**      **C<sub>2</sub>H<sub>6</sub>Cl<sub>3</sub>GeNO**ED, *ab initio*  
calculations***O*-Trichlorogermyl-*N,N*-dimethylhydroxylamine**  
*N*-Methyl-*N*-[(trichlorogermyl)oxy]methanamine**C<sub>s</sub> assumed**

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
Ge–Cl(4)	2.104(4) <sup>b)</sup>	O–Ge–Cl(4)	108.9(20)
Ge–Cl(5,6)	2.106(2) <sup>b)</sup>	Ge–O–N	104.0(11)
Ge–O	1.759(6) <sup>b)</sup>	O–N–C	106.3(9) <sup>c)</sup>
O–N	1.484(9) <sup>b)</sup>	C(7)–N–C(8)	114.1(11) <sup>c)</sup>
N–C(7)	1.447(7)	O–Ge–Cl(5,6)	111.6(12)
C(7)–H(9)	1.095(21)	N–C(7)–H(9)	108.1(10) <sup>d)</sup>
C(7)–H(10)	1.098(22) <sup>b)</sup>	N–C(7)–H(10)	106.9(11) <sup>c)</sup>
C(7)–H(11)	1.101(22) <sup>b)</sup>	N–C(7)–H(11)	110.5(11) <sup>c)</sup>
		C–N–C–H(9)	–197.5(89)
		C–N–C–H(10)	44.5(89) <sup>c)</sup>
		C–N–C–H(11)	–77.0(90) <sup>c)</sup>
		N–O–Ge–Cl(5)	58.9(37)



Local C<sub>s</sub> symmetry was assumed for the GeCl<sub>3</sub> group. The vapor was found to contain Cl<sub>3</sub>GeON(CH<sub>3</sub>)<sub>2</sub> (52(5)%) and GeCl<sub>4</sub> (48(5)%) molecules. The structural parameters of GeCl<sub>4</sub> were assumed at the values taken from the literature. The nozzle temperature was 20 °C.



<sup>a)</sup> Uncertainties were not identified, possibly estimated total errors.

<sup>b)</sup> Differences in the Ge–Cl, between the Ge–O and O–N and in the C–H bond lengths were restrained to the values from MP2/6-31G\* calculations.

<sup>c)</sup> Differences between the C–N–C and O–N–C and in the N–C–H bond angles as well as in the C–N–C–H torsional angles were restrained to the values from MP2/6-31G\* calculations.

<sup>d)</sup> Restrained to the value from MP2/6-31G\* calculations.

Losehand, U., Mitzel, N.W., Rankin, D.W.H.: J. Chem. Soc., Dalton Trans. (1999) 4291.