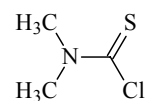
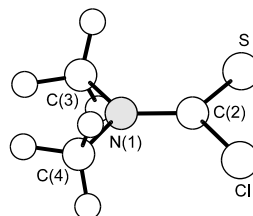


394 **C₃H₆CINS**ED, *ab initio*
calculations**Dimethylcarbamothioyl chloride****C_s**

r_g	\AA^a	θ_a	deg^a
C–H	1.118(5)	N–C=S	125.8(6)
C=S	1.652(5)	N–C–Cl	115.2 ^{b)}
N–C(2)	1.334(4)	$\Delta(\text{N–C–Cl})^c$	–10.6(13)
N–C(3,4)	1.475(3)	C(2)–N–C(3)	119.3(7)
C–Cl	1.769(5)	C(2)–N–C(4)	124.2 ^{b)}
		$\Delta(\text{C–N–C})^d$	4.9(13)
		S=C–Cl	118.9 ^{b)}
		C(3)–N–C(4)	116.2 ^{b)}
		N–C–H	107.5(9)
		τ_1^e	180 ^{f)}
		τ_2^g	0 ^{f)}

The molecular skeleton was found to be planar.

The nozzle temperature was about 80 °C.

^{a)} Three times the estimated standard errors.^{b)} Dependent parameter.^{c)} [N–C–Cl] – [N–C=S].^{d)} [C(2)–N–C(3)] – [C(2)–N–C(4)].^{e)} Torsional angle H–C(3,4)–N–C(2).^{f)} Uncertainties are not given in the original paper.^{g)} Torsional angle C(3)–N–C–S.

Naumov, V.A., Ziatdinova, R.N., Tafipolskii, M.A., Novikov, V.P.: Zh. Strukt. Khim. **41** No.3 (2000) 650; J. Struct. Chem. (Engl. Transl.) **41** (2000) 531.