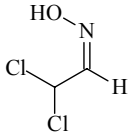
239 **$C_2H_3Cl_2NO$** **(*Z*)-Dichloroacetaldehyde oxime** **C_s** assumed

ED, *ab initio* calculations

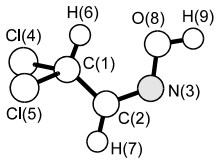


r_g	Å [a])
C(1)–C(2)	1.505
C(2)=N(3)	1.284
C(1)–Cl(4)	1.784
C(1)–Cl(5)	1.781
C(1)–H(6)	1.086
C(2)–H(7)	1.091
N(3)–O(8)	1.420
O(8)–H(9)	0.950

θ_α	deg [a])
C(1)–C(2)=N(3)	126.3
C(2)–C(1)–Cl(4)	109.0
C(2)–C(1)–Cl(5)	108.7
C(2)–C(1)–H(6)	111.1
C(1)–C(2)–H(7)	118.7
C(2)=N(3)–O(8)	112.1
N(3)–O(8)–H(9)	96.9
Cl(4)–C(1)–C(2)=N(3)	105.0 [b])
Cl(5)–C(1)–C(2)=N(3)	–132.5 [b])
H(6)–C(1)–C(2)=N(3)	0.0 [b])
H(7)–C(2)=N(3)–O(8)	–180.0 [b])
C(1)–C(2)=N(3)–O(8)	0.0 [b])
C(2)=N(3)–O(8)–H(9)	180.0 [b])

Two isomers, *E* (90(1)%) and *Z* (10(1)%), were found to be present in the gas phase. The differences between the corresponding bond lengths and bond angles between these isomers were assumed at the values from MP2 calculations. Another conformer, *Z*-II, with ΔG of *ca*. 5.5 kcal mol^{-1} from the most stable *E*-I conformer, was predicted by theoretical calculations, but the presence was not confirmed by ED or MW experiments. The nozzle temperature was *ca*. 53 °C.

[a]) Uncertainties are equivalent to those given for the *E*-isomer.
[b]) Assumed at the value from MP2/6-31G(d,p) calculations.



Kuze, N., Kitamoto, T., Usami, T., Sakaizumi, T., Ohashi, O., Iijima, K.: J. Mol. Struct. **485-486** (1999) 183.