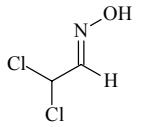
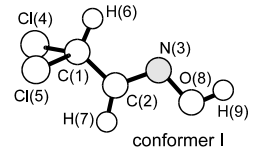
238 **$C_2H_3Cl_2NO$** **(*E*)-Dichloroacetaldehyde oxime** **C_s** assumed (conformer I)
ED, MW, *ab initio* calculations **C_1** (conformer II)

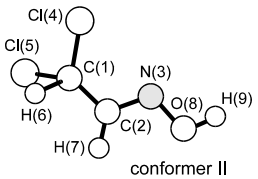


r_g	Å [a])		θ_α	deg [a])	
	conf. I	conf. II		conf. I	conf. II
C(1)–C(2)	1.497(8)	1.506	C(1)–C(2)=N(3)	117.0(8)	121.5
C(2)=N(3)	1.281(4)	1.279	C(2)–C(1)–Cl(4)	109.4(3)	113.0
C(1)–Cl(4)	1.784(2)	1.769	C(2)–C(1)–Cl(5)	109.4(3)	107.8
C(1)–Cl(5)	1.784(2)	1.794	C(2)–C(1)–H(6)	110.0 [b])	110.1
C(1)–H(6)	1.088(12)	1.090	C(1)–C(2)–H(7)	120.2 [b])	117.1
C(2)–H(7)	1.089(12)	1.091	C(2)=N(3)–O(8)	111.1(5)	110.6
N(3)–O(8)	1.415(4)	1.417	N(3)–O(8)–H(9)	97.2(50)	97.0
O(8)–H(9)	0.951(16)	0.951	Cl(4)–C(1)–C(2)=N(3)	119.7(2)	–0.4 [b])
			Cl(5)–C(1)–C(2)=N(3)	–119.7(2)	124.3 [b])
			H(6)–C(1)–C(2)=N(3)	0.0 [b])	–120.6 [b])
			H(7)–C(2)=N(3)–O(8)	0.0 [b])	0.0 [b])
			C(1)–C(2)=N(3)–O(8)	180.0 [b])	180.0 [b])
			C(2)=N(3)–O(8)–H(9)	180.0 [b])	180.0 [b])

The molecule was found by ED and MW measurements to exist as a mixture of the *Z*-isomer (10(1)%) and of the conformers I (80(1)%) and II (10(1)%) of the *E*-isomer. Their energy differences, $\Delta G°$, from *E*-I were estimated to be 1.76 and 1.36 kcal mol^{-1} for *E*-II and *Z*, respectively. The differences between the corresponding bond lengths and bond angles between the isomers and the conformers were assumed at the values from MP2 calculations. The nozzle temperature was *ca.* 53 °C.



conformer I



conformer II

[a]) Three times the estimated standard errors.
[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.

MW **C_s**

r_0	Å [a])	θ_0	deg [a])
C–Cl	1.763(19)	Cl–C–C	110.4(17)
C–H(6)	1.091 [b])	C–C–H(6)	111.5 [b])
C–C	1.504 [b])	C–C=N	116.3 [b])
C–H(7)	1.086 [b])	C–C–H(7)	120.1 [b])
C=N	1.266 [b])	C=N–O	110.7 [b])
N–O	1.408 [b])	N–O–H(9)	102.4 [b])
O–H(9)	0.956 [b])	Cl–C–C=N	117.9(26)
Cl...H(9)	5.295(51)	C=N–O–H	180.0 [b])

Atom	$\lvert a_s \rvert$ [Å]	$\lvert b_s \rvert$ [Å]	$\lvert c_s \rvert$ [Å]
Cl	1.221	1.511	0.0 [b])
H(9)	3.838	0.0 [b])	0.403

The molecule was found to have the *ac* C_s symmetry plane.

[a]) 2.5 times the estimated standard errors.
[b]) Assumed.

Usami, T., Kuze, N., Sakaizumi, T., Ohashi, O.: J. Mol. Struct. **479** (1999) 103.