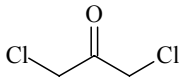
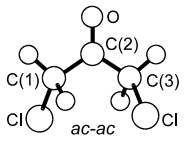
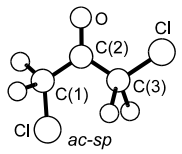
370 **$C_3H_4Cl_2O$** **1,3-Dichloro-2-propanone** **C_2** (*ac-ac*)
ED, *ab initio* calculations 1,3-Dichloroacetone **C_1** (*ac-sp*)

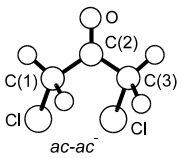


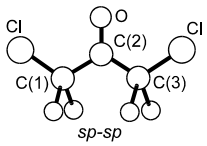
r_g	Å [a])		θ_α	deg [a])	
	ac-ac	*ac-sp*		*ac-ac*	*ac-sp*
C(1)–C(2)	1.526(3)	1.530(3)	C(1)–C(2)=O	121.0(4)	120.5(4)
C(2)–C(3)	1.526(3)	1.525(3)	C(3)–C(2)=O	121.0(4)	124.5(4)
C(2)=O	1.210(2)	1.207(2)	C(1)–C(2)–C(3)	118.0 [b])	115.0 [b])
C(1)–Cl	1.789(1)	1.786(1)	C(2)–C(1)–Cl	110.2(4)	111.6(4)
C(3)–Cl	1.789(1)	1.772(1)	C(2)–C(3)–Cl	110.2(4)	111.6(4)
C–H	1.104(8)	1.106(8)	C–C–H	113.2(21)	112.8(21)
			τ_1 [c])	116 [d])	128 [d])
			τ_2 [e])	116 [d])	12 [d])

The molecule was found to exist as a mixture of conformers. The populations of *ac-ac*, *ac-sp*, *ac-ac*$^-$ (with $\tau_1 = 127°$ and $\tau_2 = -127°$) and *sp-sp* conformers were estimated to be 66, 29, 4 and 1%, respectively. Although the ED study indicated that the potential minima corresponding to *ac-ac*$^-$ and *sp-sp* conformers may exist, the existence of these conformers is not certain because of their small populations. The C–C torsions were treated as large-amplitude vibrations. The differences between the corresponding parameters of pseudoconformers were assumed at the values from HF/6-31G(d,p) calculations. The nozzle temperature was 365 K.









[a]) Three times the estimated standard errors.
[b]) Dependent parameter.
[c]) Torsional angle O=C(2)–C(1)–Cl.
[d]) Torsional angle corresponding to the minimum of the potential energy function.
[e]) Torsional angle O=C(2)–C(3)–Cl.

Kuze, N., Kobayashi, K., Masuda, Y., Hamada, T., Sakaizumi, T., Ohashi, O., Tsuji, T., Egawa, T., Konaka, S.: J. Mol. Struct. **612** (2002) 171.