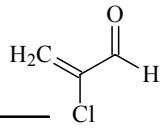
353 **C_3H_3ClO** **α-Chloroacrylaldehyde** **C_s** (*anti*)
ED, vibrational spectroscopy, *ab initio* calculations
2-Chloro-2-propenal **C_1** (near-*syn*)

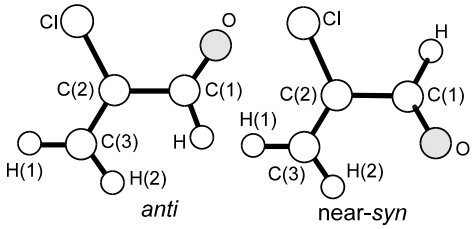


r_g	Å [a])	
	anti	near-*syn*
C(1)–C(2)	1.485(6)	1.493(6)
C=O	1.206(3)	1.208(3)
C(2)=C(3)	1.327(6)	1.324(6)
C–Cl	1.721(3)	1.732(3)
C–H [b])	1.102(12)	

θ_α	deg [a])	
	anti	near-*syn*
C–C=O	123.7(12)	121.4(12)
Cl–C(2)–C(1)	117.7(9)	116.2(9)
Cl–C(2)=C(3)	122.2(15)	122.3(15)
C(2)–C(1)–H	114.7(21)	116.9(21)
C(2)=C(3)–H(1)	119.5(51)	119.6(51)
C(2)=C(3)–H(2)	120.1(33)	118.7(33)
τ [c])	0.0 [d])	160(12)

The experimental ED data from [1] were reanalyzed. The molecule exists as a mixture of *anti* (73(4)%) and near-*syn* (27(4)%) conformers. According to results of MP2/6-31G* calculations, the *anti* form is more stable than the *syn* form by 0.3 kcal mol^{-1}. The structural differences (except for the dihedral angles) for these conformers were assumed at the MP2/6-31G* values.
The temperature of the measurements was 20°C.

[a]) Three times the estimated standard errors.
[b]) Average value.
[c]) Torsional angle C(3)=C(2)–C(1)=O; $\tau = 0°$ for the *anti* position.
[d]) Assumed.



Shishkov, I.F., Vilkov, L.V., Khristenko, L.V., Skancke, P.N.: J. Mol. Struct. **376** (1996) 103.
[1] Nipan, M.E., Sadova, N.I., Golubinskii, A.V., Vilkov, L.V.: Zh. Strukt. Khim. **27** No.2 (1986) 47; J. Struct. Chem. (Engl. Transl.) **27** (1986) 215.

Replaces II/25C (**3**, 1090)