

1503
ED

$\text{C}_4\text{H}_2\text{Cl}_2\text{O}_2$

(*E*)-1,4-Dioxo-2-butenyl dichloride
Fumaroyl dichloride

C_{2h} (*anti-anti*)

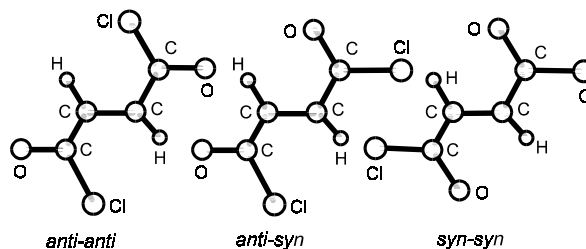
C_{2h} (*syn-syn*)

C_s (*anti-syn*)

$\text{Cl}(\text{O})\text{C}-\text{CH}=\text{CH}-\text{C}(\text{O})\text{Cl}$

r_a	\AA^a	θ_α	deg^a
C-H	1.089(25)	C-C-H	116.2 ^b
C=O	1.191(2)	C-C=C	125.2(6)
C=C	1.334(5)	C-C=O	125.5(4)
C-C	1.488(3)	C-C-Cl	114.6(3)
C-Cl	1.783(2)		

The molecule exists as a mixture of three different conformers, *anti-anti*, *anti-syn* and *syn-syn*. Approximate values for the relative energies and entropies for these three forms are 0, 0.6 and 0.7 kcal mol⁻¹, and 0, 0.7 and 0.9 cal mol⁻¹ K⁻¹. It was assumed that the three conformers have the same geometry except for the C=C-C=O torsion angles. The nozzle temperatures were 338 and 480 K. The weighted average structure is listed.



^a) Twice the estimated standard errors.

^b) Assumed.

Hagen, K.: J. Mol. Struct. **128** (1985) 139.