

1055 **C₃H₂Cl₂O₂**
ED, *ab initio* calculations
(HF/3-21G, HF/6-31G**)

r_a	\AA^a
C–C	1.498(5)
C=O	1.197(2)
C–Cl	1.772(2)
C–H	1.10 ^{b)}

Propanedioyl dichloride
Malonyl dichloride

θ_α	deg ^{a)}
C–C=O	125.8(4)
C–C–Cl	114.2(4)
Cl–C=O	120.0(6)
H–C–H	108.0 ^{b)}
C–C–C (<i>S-gauche</i>)	107.2(16)
C–C–C (<i>W-gauche</i>)	114.3 ^{c)}
C(1)–C(2)–C(3)=O(2) ^{d)}	95(6)
C(3)–C(2)–C(1)=O(1) ^{d)}	12(5)
C–C–C=O ^{e)}	115 ^{b)}

C₁ (*S-gauche*)
C₂ (*W-gauche*)
Cl(O)C–CH₂–C(O)Cl

The vapor exists as a mixture of *S-gauche* and *W-gauche* (30(15)%) conformers.
The nozzle was at 40 °C.

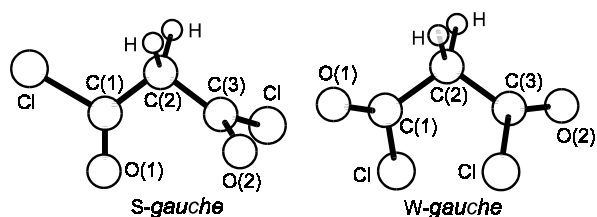
^{a)} Three times the estimated standard errors including the scale error.

^{b)} Fixed value.

^{c)} *Ab initio* value.

^{d)} Dihedral angle of the *S-gauche* conformer.

^{e)} Dihedral angles of the *W-gauche* conformer; the angles C(1)–C(2)–C(3)=O(2) and C(3)–C(2)–C(1)=O(1) are equal.



Mack, H.-G., Oberhammer, H., Della Védova, C.O.: J. Mol. Struct. **346** (1995) 51.