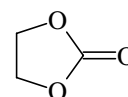


1171
MW

C₃H₄O₃

Ethylene carbonate
1,3-Dioxolan-2-one

C₂



r_0	Å ^{a)}	θ_0	deg ^{a)}
C–C	1.540 ^{b)}	O–C=O	135.8(20)
C–O	1.428(20)	C–C–O	102.4(20)
C=O	1.200 ^{b)}	C–O–C	109.5(20)
C–H	1.095 ^{b)}	O–C–O	110.4(20)

Inversion parameters

τ [deg] ^{c)}	15(2) ^{a)} ^{d)} , 19(2) ^{a)} ^{e)}
inversion barrier twisting [kJ mol ⁻¹]	2.8
inversion barrier pseudorotation [kJ mol ⁻¹]	12.9
ν_b [cm ⁻¹] ^{f)}	190

^{a)} Uncertainties were not all estimated in the original paper.

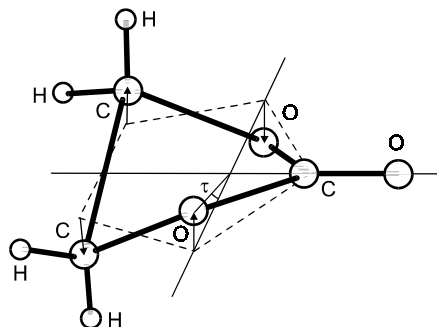
^{b)} Assumed.

^{c)} τ is the twist angle from the planar configuration (broken line), see figure.

^{d)} From the inertial data.

^{e)} Minimum of the potential function for ring twisting.

^{f)} Wavenumber of the ring-bending vibration.



Alonso, J.L., Cervellati, R., Degli Esposti, A., Lister, D.G., Palmieri, P.: J. Chem. Soc., Faraday Trans. II **82** (1986) 337.