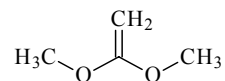


565 **C₄H₈O₂**ED, *ab initio*
calculations**1,1-Dimethoxyethene**

Ketene dimethyl acetal

C_{2v} assumed (*sp-sp*)**C₁** (*sp-ac*)

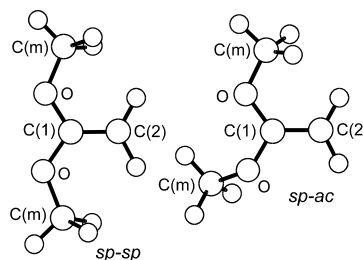
r_a	Å ^{a)}	θ_a	deg ^{a)}
C(1)=C(2)	1.333(5)	C(1)=C(2)-O	127.8(3)
C-O (mean)	1.390(2)	C(1)-O-C(m)	116.3(5)
$\Delta(\text{C-O})$ ^{b)}	0.070 ^{c)}	H-C-H	108.5(9)
C(1)-O	1.355(6)	C(1)=C(2)-H	121.4 ^{d)}
O-C(m)	1.425(6)	tilt(CH ₃) ^{e)}	3.7 ^{d)}
C-H (mean)	1.082(4)	$\tau_{1,2}$ (<i>sp-sp</i>) ^{f)}	0.0 ^{d)}
		τ_1 (<i>sp-ac</i>) ^{f)}	-4.2 ^{d)}
		τ_2 (<i>sp-ac</i>) ^{f)}	131(8)



The molecule exists as a mixture of *sp-sp* (61(7)%) and *sp-ac* (39(7)%) conformers. Local C_{3v} symmetry and staggered conformation were assumed for methyl groups. Differences between corresponding parameters of the conformers were assumed at the values from MP2/6-31G* calculations. The bond lengths and bond angles are listed for the *sp-sp* conformer.

The nozzle was at room temperature.

The energy difference between these conformers was estimated to be 0.7 kcal mol⁻¹ by HF/6-31G* and MP2/6-31G* methods.



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

^{b)} [O-C(m)] - [C(1)-O].

^{c)} Constrained to the value from MP2/6-31G* calculations.

^{d)} Assumed at the value from MP2/6-31G* calculations.

^{e)} Tilt angle of the methyl group between the C₃ axis and the O-C(m) bond direction, towards the oxygen lone pair.

^{f)} Torsional angle C(m)-O-C(1)=C(2), $\tau = 0^\circ$ for the *syn* position.

Leibold, C., Oberhammer, H.: J. Am. Chem. Soc. **121** (1999) 4852.