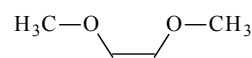


566 **C₄H₈O₂**ED, *ab initio*
calculations**(Z)-1,2-Dimethoxyethene***cis*-1,2-Dimethoxyethylene**C₁** (*sp-ap* or *sp-ac*)

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(1)=C(2)	1.332(12)	C=C-O (mean)	126.3(7)
C-O (mean)	1.391(2)	$\Delta(\text{C}=\text{C}-\text{O})$ ^{b)}	6.0 ^{c)}
$\Delta_1(\text{C}-\text{O})$ ^{d)}	0.020 ^{c)}	C(2)=C(1)-O	129.3(9)
$\Delta_2(\text{C}-\text{O})$ ^{e)}	0.076(12)	C(1)=C(2)-O	123.3(9)
C(1)-O(3)	1.343(7)	C-O-C (mean)	114.4(14)
C(2)-O(8)	1.363(7)	$\Delta(\text{C}-\text{O}-\text{C})$ ^{f)}	5.5 ^{c)}
O-C(m)	1.429(7)	C(1)-O-C(m)	117.2(15)
C-H (mean)	1.089(5)	C(2)-O-C(m)	111.7(15)
		H-C-H	110.3(16)
		C=C-H	118.1 ^{g)}
		tilt (CH ₃) ^{h)}	4.3 ^{g)}
		τ_1 ⁱ⁾	-8.5 ^{g)}
		τ_2 ^{j)}	152(6)

The experimental curves were reproduced by only one *sp-ap/ac* conformer with the conformational angle τ_2 being *ca.* 150°. MP2/6-31G* calculations predicted a *sp-ac* equilibrium structure with 134° as more stable than other possible conformers by ≥ 1.7 kcal mol⁻¹. Local C_{3v} symmetry and staggered conformation were assumed for the methyl groups.

The nozzle was at room temperature.

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

^{b)} [C(2)=C(1)-O] - [C(1)=C(2)-O].

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

^{d)} [C(2)-O] - [C(1)-O].

^{e)} [O-C(m)] - (1/2){[C(1)-O] + [C(2)-O]}.

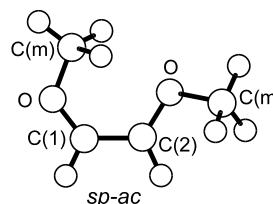
^{f)} [C(1)-O-C(m)] - [C(2)-O-C(m)].

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

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

ⁱ⁾ Torsional angle C(2)=C(1)-O-C(m), $\tau_1 = 0^\circ$ for the *syn* position.

^{j)} Torsional angle C(1)=C(2)-O-C(m), $\tau_2 = 0^\circ$ for the *syn* position.



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