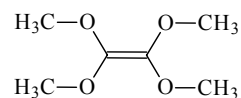


751 **C₆H₁₂O₄**ED, *ab initio*
calculations**Tetramethoxyethene**

Ethenedione bis(dimethyl acetal)

D₂ assumed (*ac-ac-ac-ac*)

r_a	\AA^a	θ_a	deg^a
C(1)=C(2)	1.335(5) ^{b)}	C=C-O	121.5(3)
C(1,2)-O	1.361(4)	C-O-C	115.8(7)
O-C(methyl)	1.430(5)	H-C-H	109.7(8)
C-H	1.099(4)	tilt(CH ₃) ^{c)}	2.3(22)
		τ_1^d	108.5(12)
		τ_2^e	13.5(30)

Local C_{3v} symmetry and staggered conformation were assumed for methyl groups. The ED results agreed with the presence of only one all-*ac* D₂ conformer, which was also predicted by HF/6-31G* and MP2/6-31G* calculations to be more stable than other possible conformers by $\geq 1.5 \text{ kcal mol}^{-1}$.

The nozzle was at 36 °C.

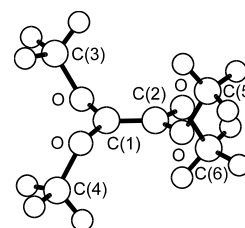
^{a)} Three times the estimated standard errors including a systematic error.

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

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

^{d)} The C=C-O-C torsional angle from the *syn* position.

^{e)} Torsional angle around the C(1)=C(2) bond; a positive value means that the C(3)...C(6) and C(4)...C(5) distances increase.



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