

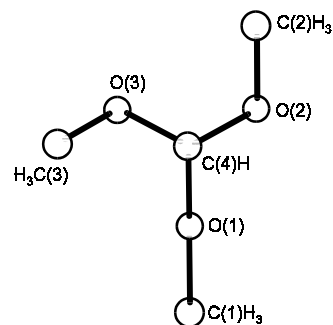
**1824**     **C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>**  
ED, *ab initio* (STO-3G)  
and MM calculations

**Trimethoxymethane**

**C<sub>1</sub>**  
HC(OCH<sub>3</sub>)<sub>3</sub>

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C(4)–O	1.382(6)	O(1)–C(4)–O(3)	115.0(10)
C(1,2,3)–O	1.418(6)	O(1)–C(4)–O(2) <sup>b)</sup>	109.2(6)
C–H	1.112(1)	C–O–C	114.3(6)
		O–C(1,2,3)–H	109.9(3)
		$\tau_1$ <sup>c)</sup>	57(1)
		$\tau_2$ <sup>d)</sup>	60(3)
		$\tau(\text{CH}_3)$ <sup>e)</sup>	68(6)

The molecule was found to exist almost exclusively as an asymmetric all-staggered TGG conformer. The structure is adequately reproduced by molecular mechanics calculations. The nozzle temperature was 27 °C.



<sup>a)</sup> Estimated standard errors.

<sup>b)</sup> Assumed equal to angle O(3)–C(4)–O(2).

<sup>c)</sup> Dihedral angle C(1)–O(1)–C(4)–O(3), assumed equal to C(3)–O(3)–C(4)–O(1).

<sup>d)</sup> Dihedral angle C(2)–O(2)–C(4)–O(3).

<sup>e)</sup> Zero position for the eclipsed conformation.

Spelbos, A., Mijlhoff, F.C., Faber, D.H.: J. Mol. Struct. **41** (1977) 47.