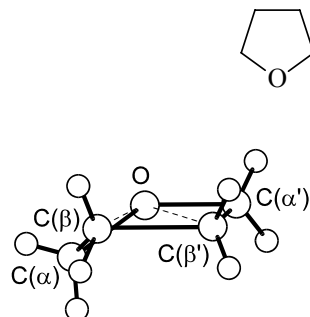


563
MW C_4H_8O

Tetrahydrofuran

 C_{2v}
(effective symmetry class)
(pseudorotation)

$r_0^a)$	$\text{\AA}^b)$	$\theta_0^a)$	$\text{deg}^b)$
O...C(β)	2.3512(22)	ϕ	52.50(13)
O...C(β')	2.4032(23)	$\rho^c)$	41.22(40)
C(β)–C(β')	1.53324(69)	$\tau^d)$	40.86(39)
C(α)–C(β)	1.5239(26)	$\tau'^e)$	–5.38(12)
C(α')–C(β')	1.5519(27)		
C(α)–H(ax)	1.1047(47)		
C(α)–H(eq)	1.0853(47)		
C(α')–H(ax)	1.09628(60)		
C(α')–H(eq)	1.09372(60)		
C–O	1.427 ^{f)}		
C(β)–H, C(β')–H	1.095 ^{f)}		



Equilibrium configuration.

Two pseudorotation vibrational spacings have been measured directly to be $\Delta E_{01} = 21307.71(3)$ MHz and $\Delta E_{23} = 61205.69(3)$ MHz. They have been used, together with the lowest 10 measured far-IR transition frequencies and with the effective moments of inertia of the ground state and their shifts upon excitation observed, to determine the potential energy function for pseudorotation and the associated structural relaxations. The potential energy barriers are 45 cm^{-1} at the envelope conformation of the oxygen and 16 cm^{-1} at the twisted conformation of the C(β)–C(β') bond relative to the C(α)OC(α') plane. The four symmetrically equivalent equilibrium structures are close to the envelope conformations of the CH_2 groups next to the oxygen atom. While the C–O bond lengths and the local CH_2 angles appear to remain unaffected by pseudorotation, significant changes found for the diagonal O...C distances as well as for the C–C and C–H bond lengths suggest possible effects of hyperconjugation.

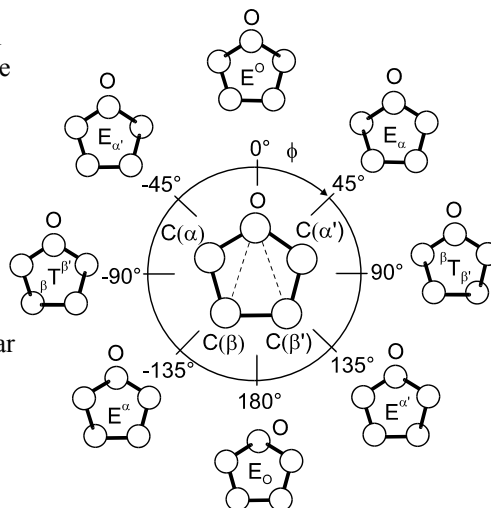


Figure displays pseudorotation. The principal a axis coincides with the C_2 axis and the b axis is within the plane of the non-puckered ring (center). Envelope (E) conformations are characterized by coplanarity of four adjacent ring atoms, and twisted conformations (T) by coplanarity of three adjacent ring atoms and the midpoint between the opposite bond. The indices refer to ring atoms above (superscript) or below (subscript) the a, b plane. The pseudorotation angle ϕ is associated with the ring conformation. The substitution of ϕ by $-\phi$ and by $\phi + 180^\circ$ correspond to the reflection at the a, c and a, b planes, respectively.

^{a)} Structural parameters at the equilibrium pseudorotation configuration.

^{b)} Estimated standard errors.

^{c)} Puckering amplitude.

^{d)} Angle by which the C(α)C(β)O plane is bent down from the C(β)OC(β') plane.

^{e)} Angle by which the C(α')C(β')O plane is bent up from the C(β)OC(β') plane.

^{f)} Assumed.

Meyer, R., López, J.C., Alonso, J.L., Melandri, S., Favero, P.G., Caminati, W.: J. Chem. Phys.
111 (1999) 7871.

[II/25C \(3, 1745\)](#)