

Conformational Analysis of $C_mH_{2m+1}OCH_2CH_2OH$ ($m = 1-4$): The Role of $CH\cdots O$ Intramolecular Interactions

Francisco P. S. C. Gil,[†] A. M. Amorim da Costa,[‡] and J. J. C. Teixeira-Dias^{*,‡}

Molecular Physical Chemistry Research Unit, Departments of Chemistry and Physics, University of Coimbra, P-3049 Coimbra, Portugal

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Structures and energies of the more stable conformations of $C_mH_{2m+1}OCH_2CH_2OH$ (C_mE_1 , $m = 1-4$) have been determined by gradient geometry refinement at *ab initio* level. For $m = 3$ (C_3E_1) and $m = 4$ (C_4E_1), the results show that attractive $CH\cdots O$ intramolecular interactions associated with the formation of five-membered rings in the alkylic fragments of these molecules lead to the stabilization of *gauche* arrangements in the $CC-CO$ axes. Since these $CH\cdots O$ interactions compete, in energy terms, with conformational effects, they are found to have important structural consequences. In addition, the formation of five-membered rings closed by $CH\cdots O$ and $OH\cdots O$ contacts gives rise to vibrational couplings in the $C(H_2)tOtC(H_2)$ moieties and to conformationally sensitive vibrations.

1. Introduction

Molecules with the general formula $C_mH_{2m+1}(OCH_2CH_2)_nOH$, abbreviated C_mE_n , display a wide range of interesting properties and aggregation patterns both in van der Waals clusters^{1,2} and in condensed phase.³⁻⁷ In short, these characteristics result from interplay of (i) the relative importance of the polar and nonpolar fragments, (ii) conformational degrees of freedom, (iii) the occurrence of intramolecular hydrogen bonding type of interactions, and (iv) the extent of intermolecular interactions, hydrogen bonding included. While C_mE_n compounds have been widely studied by various experimental methods,¹⁻⁷ an assessment of the relative importance of conformational effects and hydrogen bonding type of interactions at the unimolecular and oligomer levels is still lacking.

The two more stable conformers of C_1E_1 correspond to the *tgg'* and *ggg'* forms, *tgg'* being 6–7 kJ mol⁻¹ more stable than *ggg'*.⁸ These conformers, which owe their stability mainly to $O\cdots H-O$ intramolecular hydrogen bonds, are associated with a relatively sharp spectral feature occurring at *ca.* 3608 cm⁻¹ in the FTIR and Raman spectra of sufficiently diluted solutions in CCl₄. This feature is ascribed to ν_{OH} in monomeric species and becomes progressively prominent at lowering concentrations of C_1E_1 .⁸ In addition, structures and vibrational frequencies of the relevant hydrogen-bonded dimers of C_1E_1 have been previously studied by an *ab initio* method.⁹

A comparison of the performances of various *ab initio* calculations carried out for the structures and conformational energies of C_1E_1 led to the general conclusion that a 3-21G basis set to which polarization functions were deliberately added to describe the lone pair "tail" functions of the second period atoms—basis set hereafter named as 3-21G*—is the smallest basis set that reproduces adequately the structures and energies of the more relevant conformers, as these are given by a MP2/6-31G* calculation.¹⁰ Based on this conclusion and on additional evidence hereafter presented concerning the suitability of the 3-21G* basis set for dealing with $CH\cdots O$ interactions in $CH_3CH_2CH_2OCH_3$ and C_3E_1 , the structures and relevant conformations of C_mE_1 ($m = 1-4$) are now determined by *ab initio*

calculations at the 3-21G* level, and the corresponding *ab initio* harmonic force fields are used to calculate the Raman spectra for the studied compounds.

2. Methods

Ab initio MO calculations were carried out with the *Gaussian 92* program system,¹¹ using a 3-21G* basis set which included *d* functions ($\zeta = 0.8$) deliberately added to the C and O atoms. In addition, calculations at the MP2/6-31G*/3-21G* level have been also carried out for C_3E_1 and $CH_3CH_2CH_2OCH_3$. The errors in bond lengths and bond angles are less than 1 pm and 0.1°, respectively, and the stopping criterion for the SCF iterative process required a density matrix convergence of less than 10⁻⁸. Calculation of normal modes of vibration and their frequencies was carried out by the above mentioned program, using the *ab initio* derived force fields. Visual inspection of the normal modes of vibration was carried out using the Molecular Editor program.¹²

The population of each conformational level is estimated by the Boltzmann factor $w_i^* \exp(-\Delta E/RT)$, where w_i is the statistical weight and ΔE refers to the difference in energy of the minima at which two conformers are defined. The calculated spectra at a particular temperature are obtained by the superposition of the spectra of the individual conformers weighted by the corresponding Boltzmann population factors.

The compounds were obtained from Aldrich, and the Raman spectra of the pure samples were recorded on a Spex 1403 model, 0.85 m double spectrometer, with a 514.5 nm line of an argon ion laser (Spectra-Physics, Model 2020-03) used as Raman excitation. Under the experimental conditions, the estimated frequency error is approximately ± 1 cm⁻¹.

Figure 1 represents schematically the more stable conformers of C_mE_1 ($m = 1-4$), identified by a letter acronym which specifies the dihedral arrangements involving skeletal atoms. For example, the more stable conformer of C_4E_1 is labeled *tgttgg'*, following a left-to-right order of the dihedral axes in $CCtCgCtOtCgCg'OH$, where *t*, *g*, and *g'* designate *trans*, *gauche*, and *gauche'* conformations, respectively.

3. Results and Discussion

Methoxyethanol (C_1E_1). Starting with C_1E_1 , the intramolecularly hydrogen-bonded conformers, *tgg'* and *ggg'*, account

[†] Department of Physics.

[‡] Department of Chemistry.

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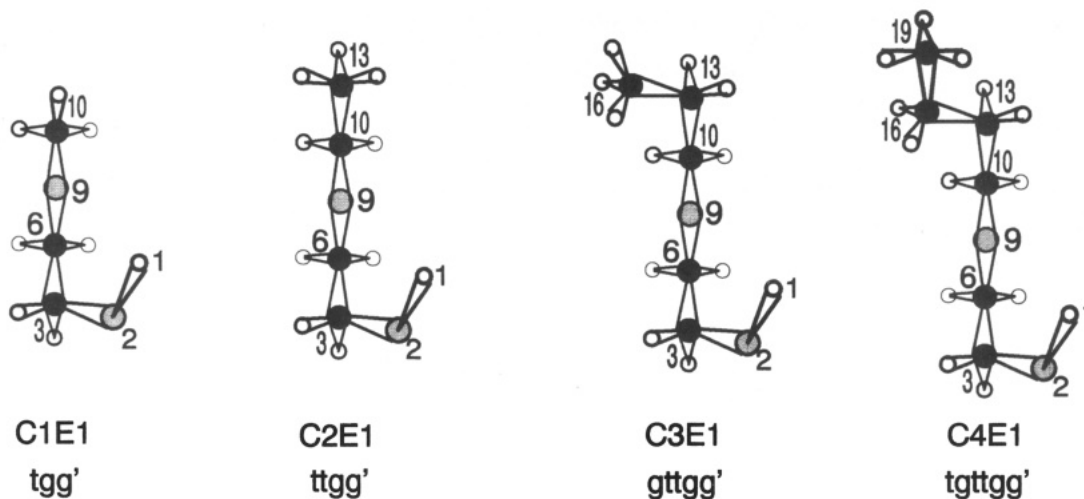


Figure 1. Numbering of atoms for the most stable conformers of C_mE_1 ($m = 1-4$) (schematic).

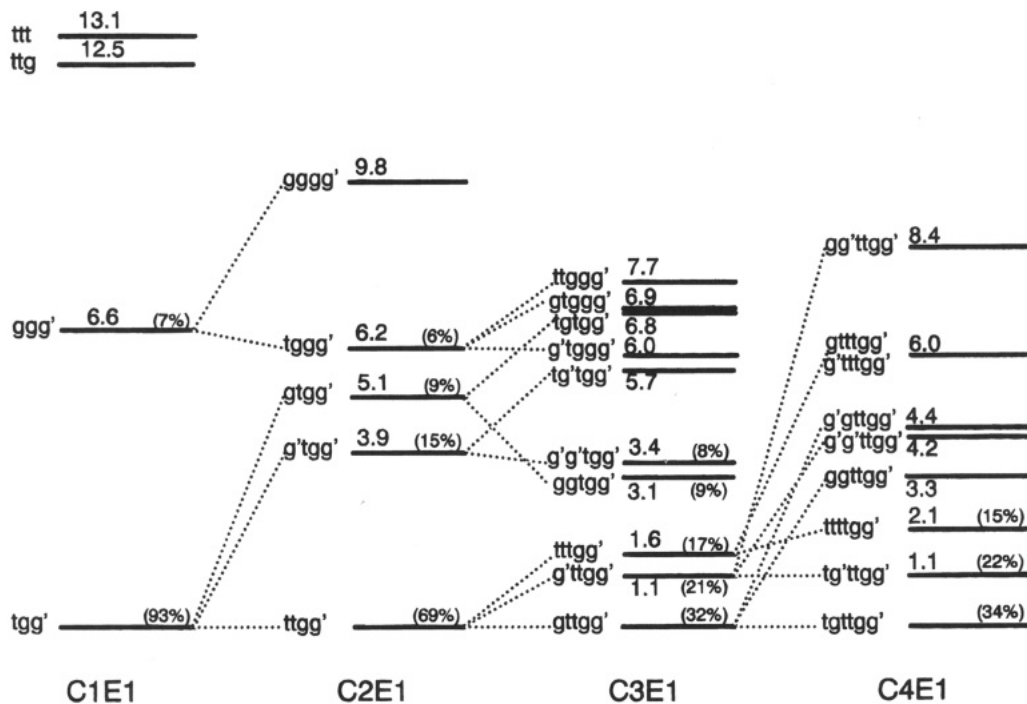


Figure 2. Correlation diagram for relevant conformational states of C_mE_1 ($m = 1-4$), with energy differences (kJ mol^{-1}) and Boltzmann populations at room temperature shown.

for more than 99% of the total population, *i.e.*, the Boltzmann population of all conformers (Figure 2). As it was previously shown,¹ the structures of these conformers owe their stability mainly to O—H—O intramolecular hydrogen bonds which give rise to five-membered configurations like the one schematically represented in Figure 3b.

Ethoxyethanol (C_2E_1). Substitution of one methyl H atom of the "parent" molecule C_1E_1 by a new methyl group leads to one of three different conformations. In particular, the more stable conformer of C_1E_1 , tgg' , gives rise to three C_2E_1 conformers, namely, $ttgg'$, $g'tgg'$, and $gtgg'$, which account for *ca.* 93% of the total population (Figure 2). As expected, the $ttgg'$ conformer is the more stable form of C_2E_1 , since the methyl group in the *trans* position is not sterically hindered by the H atoms of $C_{(6)}H_2$ (see Figure 1). For $g'tgg'$, the methyl group is on the opposite side of the CO—CC axis with respect to the OH group, whereas for $gtgg'$ the methyl group is on the same side of hydroxyl group (Figure 4) This structural feature enables us to understand the stability of $g'tgg'$ with respect to $gtgg'$ (the $gtgg'-g'tgg'$ energy difference is *ca.* 1 kJ mol^{-1} , Figure 2).

The three conformers of C_2E_1 which correlate with tgg' have lower energy than the more stable form resulting from ggg' (Figure 2). While this conformer originates three conformations for C_2E_1 , namely, $tggg'$, $gggg'$, and $g'ggg'$, only the first two are stable, since $g'ggg'$ does not correspond to an energy minimum, presumably due to strong steric hindrance between the H atoms of the CH_3 and $C_{(3)}H_2$ groups.

Figure 5 presents the calculated *vs* experimental Raman spectra of C_2E_1 , at 158 and 298 K. At these temperatures, the most stable conformer, $ttgg'$, is found to contribute *ca.* 93% and 69% of the total population, respectively. Hence, at room temperature, 30% of the total population is collectively ascribed to the $g'tgg'$, $gtgg'$, and $tggg'$ conformers. As it can be seen from Figure 5, C_2E_1 gives rise to a Raman spectrum whose temperature dependence is due to the occurrence of low-lying conformational states that significantly contribute to the overall population even at room temperature, a behavior not found for C_1E_1 .

While the experimental spectra were obtained in the pure liquid, *i.e.*, with strongly interacting molecules, the calculated

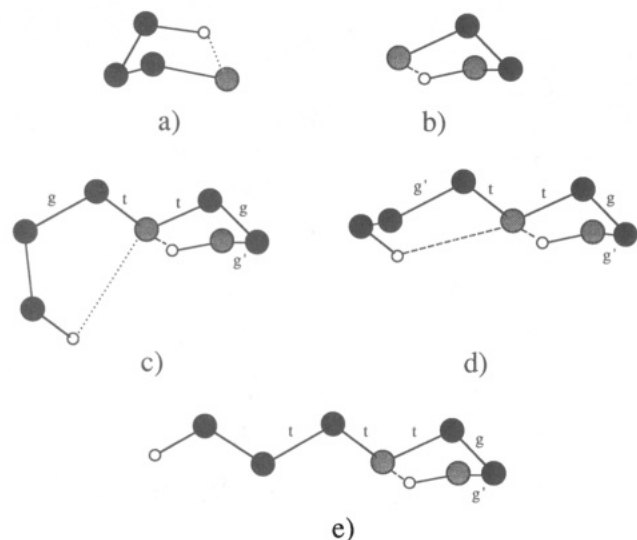


Figure 3. Conformations of five-membered rings with "envelope" conformation related to intramolecular hydrogen bonding formation: (a) C–H···O hydrogen bond, (b) O–H···O hydrogen bond, (c) $gtgg'$, (d) $g'ttgg'$, and (e) $ttgg'$ conformers of C_3E_1 . Only hydrogen atoms which are directly involved with hydrogen bonding are shown.

spectra were obtained for the one-molecule situation. Hence, the calculated and the experimental spectra should not be compared at a particular temperature (the agreement is not particularly good), but the comparison should be made instead between the trends revealed by the calculated and the experimental spectra at different temperatures. This reasoning relies on the assumption that the vibrational modes in the more conformationally sensitive region are not expected to be particularly sensitive to averaged nonspecific intermolecular interactions. In fact, the *ab initio* calculated spectra qualitatively reproduce the experimental trends observed on temperature variation, in particular, for the relative intensities of bands in regions A (*vs* A'), B (*vs* B'), and C (*vs* C') at 298 K (*vs* 158 K) (Figure 5).

Propoxyethanol (C_3E_1). The C_3E_1 conformers which correlate with the more stable conformer of C_2E_1 , *i.e.*, $gttgg'$, $g'ttgg'$, and $tttgg'$, lay below the value of RT at room temperature (≈ 2.5 kJ mol⁻¹) and together account for 70% of the total population (Figure 2). Surprisingly, the two more stable forms, $gttgg'$ and $g'ttgg'$, do not adopt an *all-trans* conformation in the propyl fragment (CC–C–) but exhibit instead gt and $g't$ conformations, respectively. Interestingly, this trend is also found for the propyl moiety of $CH_3CH_2CH_2OCH_3$. In fact, calculations performed for this molecule yielded gt as the more stable conformer (this conformer corresponds to $CCgCtOC$) and tt and gg as the second and third more stable conformers,¹³ as can be seen by the following results (see Figure 2).

	$\Delta E/kJ\ mol^{-1}$		
	$gt(tgg')$	$tt(tgg')$	$gg(tgg')$
$CH_3CH_2CH_2OCH_3$	0.0	1.8	4.9
C_3E_1	0.0	1.6	3.1

This order of relative stability of conformers suggests the occurrence, for both molecules, of weak CH···O attractive interactions¹⁴ associated with the terminal methyl C atom of the propyl fragment and the formation of five-membered rings (see Figure 3a). These CH···O contacts stabilize the *gauche* with respect to the *trans* conformation in the CC–CO axis. Their occurrence has been previously reported,^{15–17} and in spite of their very low strength, they have important structural implications,¹⁸ as herein illustrated for $CH_3CH_2CH_2OCH_3$ and C_3E_1 .

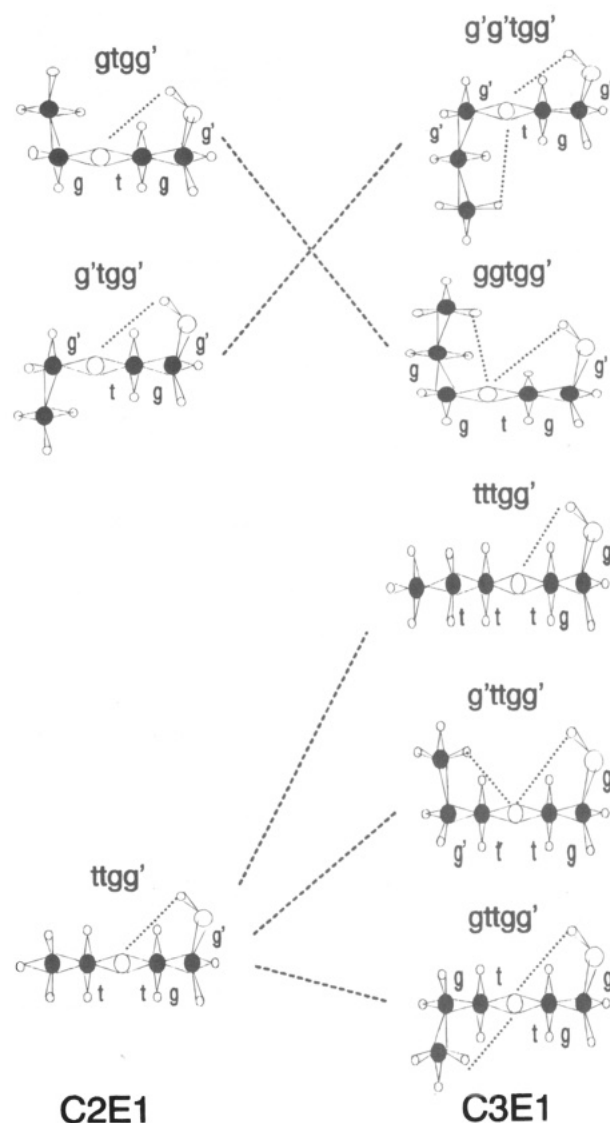


Figure 4. Geometries of the more stable conformers of C_2E_1 and C_3E_1 (schematic).

By comparison of the conformational energy differences for these two molecules, it is worth pointing out that the $tt - gt$ energy difference in the ether is close to the $tttgg' - gttgg'$ corresponding value for C_3E_1 , but the $gg - gt$ difference in the ether is appreciably larger than the corresponding value for C_3E_1 . This is due to nonbonded atom repulsions between H atoms of the methyl group adjacent to the O atom and of the C_β -methylene group of the propyl fragment. Of course, for $CH_3CH_2CH_2OCH_3$, the stabilizing effect of an intramolecular OH···O hydrogen bond does not occur.

Considering now the geometrical parameters (contact distances and angles at the contact H atom) related to the CH···O contacts in these two molecules, one concludes that they fall

	$gt(tgg')$	$gg(tgg')$
$CH_3CH_2CH_2OCH_3$		
CH···O distance/pm	253	258
CH···O angle/deg	97	97
C_3E_1		
CH···O distance/pm	254	259
CH···O angle/deg	97	96

within the range considered to be acceptable for a CH···O hydrogen bonding type of interaction.¹³ In addition, one should

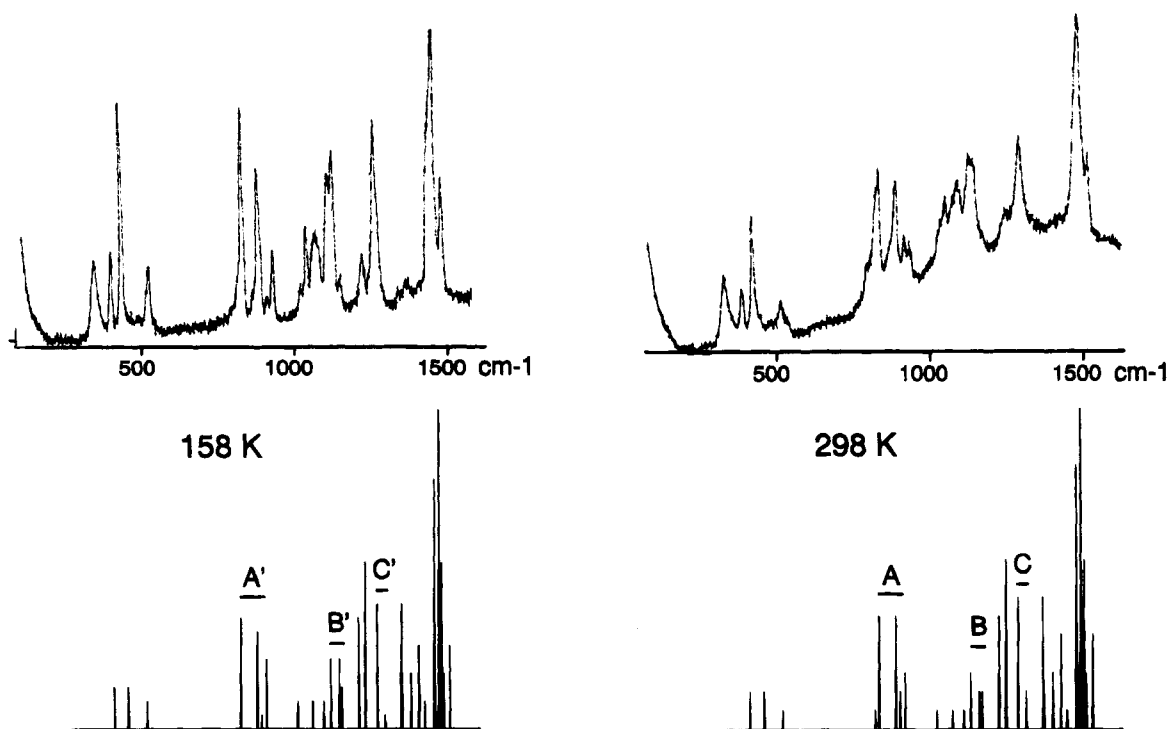


Figure 5. Calculated vs experimental Raman spectra of pure C_2E_1 at 158 and 298 K. The calculated spectra represent contributions of the various conformers weighted by their Boltzmann populations. A scaling factor of 0.889, applied to the calculated frequencies, enabled adjustment of the calculated frequencies to the observed values.

note that the $H_{\text{contact}}CC$ angle is *ca.* 1° smaller for $gttg'g'$ than that for $tttg'g'$, and the contact H atom is *ca.* 0.02 charge units more positive in the first conformer.

For C_3E_1 , the $gttg'g'$ form is more stable than $g'ttg'g'$, since for the first of these conformers, the methyl group is on the opposite side of the $CCtO_tCC$ axis, whereas for $g'ttg'g'$, the methyl group is on the same side of this dihedral axis (Figure 4). Hence, for the former structure, the $CH=O$ and $OH=O$ interactions involve different lone pairs of the ether-type O atom and the contact H atoms are not close enough for interaction, whereas for $g'ttg'g'$, the same O lone pair is shared by both hydrogen bonding interactions and the contact H atoms are close enough to repel each other (Figure 4). In fact, for the $g'ttg'g'$ conformer, the $OH=O$ and $CH=O$ contact distances are larger, by *ca.* 3 and 5 pm, respectively, than the corresponding distances for $gttg'g'$, thus suggesting weaker $OH=O$ and $CH=O$ interactions for $g'ttg'g'$ (the $g'ttg'g' - gttg'g'$ energy difference is ≈ 1 kJ mol $^{-1}$, Figure 2).

The occurrence of highly populated conformers with different molecular shapes and volumes impose distinct packing constraints on cooling. In addition, if their barriers for interconversion are high, a nonequilibrium situation is attained on cooling and a supercooled liquid obtained. This behavior has been previously found for C_mE_1 when $m = 2, 3$, and 4.⁵

Considering the case of C_3E_1 , the barrier heights between its three more stable and highly populated conformational states ($gttg'g'$, $g'ttg'g'$, and $tttg'g'$) have been evaluated within the rigid rotor approximation and yield the following values:

$$\Delta E/kJ\ mol^{-1} \quad \begin{array}{ccc} g'(ttg'g') \rightarrow t(ttg'g') & t(ttg'g') \rightarrow g'(ttg'g') & g'(ttg'g') \rightarrow g'(ttg'g') \\ 22 & 20 & 24 \end{array}$$

While geometry relaxation is expected to reduce these values, it is likely that the corrected values should still be much larger than RT at room temperature, preventing the corresponding conformational transitions from occurring at lower temperatures. Hence, annealing is not expected to be much efficient in

TABLE 1: Calculated (3-21G*) Nonscaled Frequencies (cm $^{-1}$) and Raman Intensities (in Parentheses) for the Three More Stable Conformers of C_3E_1 ^a

approx description	$gttg'g'$	$g'ttg'g'$	$tttg'g'$
ν_{OH}	3968 ₍₄₁₎	3974 ₍₄₈₎	3968 ₍₄₁₎
ν_{CH_3} as A'	3272 ₍₂₉₎	3268 ₍₂₉₎	3245 ₍₂₉₎
ν_{CH_3} as A''	3240 ₍₅₆₎	3242 ₍₅₇₎	3246 ₍₅₃₎
ν_{CH_3} s	3187 ₍₉₈₎	3188 ₍₆₀₎	3183 ₍₁₀₀₎
$\nu_{C_{13}H_2}$ s	3194 ₍₁₁₀₎	3195 ₍₁₃₉₎	3197 ₍₇₁₎
δ_{CH_3} as A'	1660 ₍₁₆₎	1659 ₍₁₁₎	1658 ₍₁₎
δ_{CH_3} as A''	1648 ₍₂₄₎	1648 ₍₂₂₎	1653 ₍₂₀₎
$\delta_{C_{13}H_2}$	1627 ₍₁₈₎	1626 ₍₁₉₎	1641 ₍₃₀₎
δ_{CH_3} s	1556 ₍₃₎	1556 ₍₂₎	1563 ₍₂₎
$\omega_{C_{13}H_2}$	1505 ₍₂₎	1507 ₍₀₎	1457 ₍₂₎
$t_{C_{13}H_2}$	1432 ₍₁₇₎	1434 ₍₁₅₎	1446 ₍₂₁₎
$\gamma_{CH_3} A'/\gamma_{C_{10}H_2}$	1284 ₍₄₎	1283 ₍₃₎	1296 ₍₃₎
$\gamma_{CH_3} A''/\gamma_{C_{10}H_2}$	1018 ₍₁₎	1012 ₍₁₎	982 ₍₂₎
$\nu_{C_{13}C_{16}}/\nu_{C_{10}C_{13}}$	937 _{(9)/1145₍₃₎}	934 _{(8)/1145₍₃₎}	1096 ₍₈₎

^a For the numbering of atoms see Figure 1.

inducing equilibria between conformers. In addition, since these conformers have different shapes and volumes, crystalline solids of C_3E_1 are difficult to obtain on cooling.

The second and third more stable conformers of C_2E_1 , $g'ttg'g'$ and $gttg'g'$, give rise to three C_3E_1 conformations each. However, the $gg'ttg'g'$ and $g'ttg'g'g'$ forms do not originate stable conformations, presumably due to strong steric hindrances between the H atoms of the CH_3 and $C_{10}H_2$ groups, a trend already found for the $g'gg'g'$ form of C_2E_1 .

Table 1 presents the approximate descriptions of some of the calculated nonscaled frequencies and their Raman intensities for the three more stable conformers of C_3E_1 ($gttg'g'$, $g'ttg'g'$, and $tttg'g'$).

From this table, a general trend emerges showing that the vibrational modes whose frequencies are more sensitive to conformation present a $tttg'g'$ frequency appreciably different from the $gttg'g'$ and $g'ttg'g'$ frequencies which, in turn, are close to one another. In particular, ν_{CH_3} as A', $\delta_{C_{13}H_2}$, $\omega_{C_{13}H_2}$, and $t_{C_{13}H_2}$ present a $tttg'g'$ frequency appreciably shifted from the

TABLE 2: Calculated (3-21G*) Contact Distances, Angles, and Mulliken Charges for the Three More Stable Conformers of C₃E₁^a

	g'ttgg'	g'ttgg'	tttgg'
Distances/pm			
(O)H··O	217	220	217
(C)H··O	254	259	
Angles/deg			
OH··O	113	111	113
CH··O	97	96	
CCH··(O)	110	110	111
Mulliken Charges/e			
O ₍₉₎	-0.70	-0.70	-0.71
C ₍₁₀₎	0.01	0.01	0.02
C ₍₁₆₎	-0.62	-0.62	-0.63
(C)H··(O)	0.23	0.22	0.22

^a For the numbering of atoms see Figure 1.

mean value of the g'ttgg' and g'ttgg' frequencies ($\Delta\nu/\text{cm}^{-1} = -25, 15, -51, \text{ and } 13$, respectively). This trend is exhibited also by the Mulliken charges on the ether O atom and on the α and γ C atoms of the propyl fragment. In fact, the charge values of these atoms for the *trans* conformer are different from the charges for the *gauche* conformers which, in turn, are very close to one another (Table 2).

Considering now the first of the above mentioned vibrations (ν_{CH_3} as A'), its visual inspection in the various conformers, using the Molecular Editor program,¹² indicates that the CH oscillator directly involved in the CH··O interactions which occur for the g'ttgg' and g'ttgg' conformers becomes distinct from the other two CH oscillators as it exhibits a much larger vibrational amplitude. Probably this effect results from the fact that the H contact atom is subject to the attraction of the negative ether O atom and so is being pulled in that direction.

It is also worth pointing out that $\nu_{\text{C}_{(13)}\text{C}_{(16)}}$ and $\nu_{\text{C}_{(10)}\text{C}_{(13)}}$ split into two distinct frequencies in the *gauche* conformers and give rise to a single frequency in the *trans* form.

Not surprisingly, for ν_{OH} , the conformer which is singled out is g'ttgg', not tttgg', since this vibrational frequency follows the pattern observed for the geometrical parameters of the OH··O contact, namely, its contact distance and angle (Table 2).

Visual inspection of the vibrations using Molecular Editor¹² enables us to conclude that coupling of vibrations on distinct intramolecular rings is mainly brought about by vibrations localized in the central part of the molecule, *i.e.*, in the C_tO_tC axis, namely, C—O and O—C stretchings, twisting, and rocking modes. A mixture of these coordinates makes the resulting variations conformation dependent, an effect which was previously noticed for polymer chains⁷ and spectroscopically observed also for the CH oscillations of the methylene groups adjacent to the central ether-type O atom.²⁰ In general and qualitative terms, the extent of this vibrational mixing for C₃E₁ increases along this series tttgg' < g'ttgg' < g'ttgg', being larger for g'ttgg' since for this conformer both five-membered rings lay on the same side of the CC_tO_tCC plane (Figure 3).

Butoxyethanol (C₄E₁). For C₄E₁, only the conformations resulting from the three more stable "parent" conformers of C₃E₁ were considered, and their structures were determined. The three more stable conformers of C₄E₁, *i.e.*, tttgg', g'ttgg', and tttgg', account for 71% of the total population (Figure 2). For

all the conformers considered herein and a particular "parent" conformation of C₃E₁, the order of increasing conformational energy leads to the *trans* being more stable than *gauche* conformations for the new dihedral angle CC—CC (Figure 2). This stresses the importance of five-membered ring geometries (Figure 3) for the formation of attractive intramolecular C—H··O interactions. In fact, conformers with a CH··O interaction forming a five-membered ring (*i.e.*, tttgg' and g'ttgg') are more stable than those which exhibit the same type of interaction but give rise to a six-membered ring (*i.e.*, g'ttgg' and g'ttgg'). For these less stable conformers, the angles C₁₉C₁₆C₁₃, C₁₆C₁₃C₁₀, and C₁₃C₁₀O₉ are *ca.* 2° larger than those for the former ones.

Conformers g'ttgg' and g'ttgg' form five-membered rings through a CH··O interaction, but the possible steric repulsion between the CH₃ group and other parts of the molecule determines their lower relative stability with respect to the three more stable conformers. The angles C₁₉C₁₆C₁₃, C₁₆C₁₃C₁₀, and C₁₃C₁₀O₉ for those conformers are *ca.* 1° larger than those for the first two conformers, tttgg' and g'ttgg'.

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