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A Density Function Theory Based Comparative Study of Trans and Cis - Resveratrol

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Abstract : Resveratrol (RvL), a phenolic compound, is a key ingredient in wine and tomatoes that has been studied over the years because of its important bioactivities such as anti-oxidant, anti-aging and antimicrobial properties. Out of the two isomeric forms of resveratrol i.e. trans and cis, the health benefit is primarily associated with the trans form. Thus, studying the structural properties of the isomers will not only provide an insight into understanding the RvL isomers, but will also help in designing parameters for differentiation in order to achieve 99.9% purity of trans-RvL. In the present study, density function theory (DFT) study is conducted, using the B3LYP/6-311++G** model to explore the through bond and through space intramolecular interactions. Properties such as vibrational spectroscopy (IR and Raman), nuclear magnetic resonance (NMR) spectra, excess orbital energy spectrum (EOES), energy based decomposition analyses (EDA) and Fukui function are calculated. It is discovered that the structure of trans-RvL, although it is C1 non-planar, the backbone non-H atoms are nearly in the same plane; whereas the cis-RvL consists of two major planes of R1 and R2 that are not in the same plane. The absence of planarity gives rise to a H-bond of 2.67Å in cis-RvL. Rotation of the C(5)-C(8) single bond in trans-RvL produces higher energy barriers since it may break the (planar) entire conjugated structure; while such rotation in cis-RvL produces multiple minima and maxima depending on the positions of the rings. The calculated FT-IR spectrum shows very different spectral features for trans and cis-RvL in the region 900 – 1500 cm-1, where the spectral peaks at 1138-1158 cm-1 are split in cis-RvL compared to a single peak at 1165 cm-1 in trans-RvL. In the Raman spectra, there is significant enhancement of cis-RvL in the region above 3000cm-1. Further, the carbon chemical environment (13C NMR) of the RvL molecule exhibit a larger chemical shift for cis-RvL compared to trans-RvL (Δδ = 8.18 ppm) for the carbon atom C(11), indicating that the chemical environment of the C group in cis-RvL is more diverse than its other isomer. The energy gap between highest occupied molecular orbital (HOMO) and the lowest occupied molecular orbital (LUMO) is 3.95 eV for trans and 4.35 eV for cis-RvL. A more detailed inspection using the recently developed EOES revealed that most of the large energy differences i.e. Δεcis-trans > ±0.30 eV, in their orbitals are contributed from the outer valence shell. They are MO60 (HOMO), MO52-55 and MO46. The active sites that has been captured by Fukui function (f + > 0.08) are associated with the stilbene C=C bond of RvL and cis-RvL is more active at these sites than in trans-RvL, as cis orientation breaks the large conjugation of trans-RvL so that the hydroxyl oxygen’s are more active in cis-RvL. Finally, EDA highlights the interaction energy (ΔEInt) of the phenolic compound, where trans is preferred over the cis-RvL (ΔΔEi = -4.35 kcal.mol-1) isomer. Thus, these quantum mechanics results could help in unwinding the diversified beneficial activities associated with resveratrol.

Keywords : resveratrol, FT-IR, Raman, NMR, excess orbital energy spectrum, energy decomposition analysis, Fukui function
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