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# Geometric, energetic and topological analysis of $(ethanol)_8$-water heterononamers: A computational approach

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This research focused on the computational study of intermolecular interactions responsible for the geometric preferences and stability of $(ethanol)_8$-water heterononamers. The B3LYP functional was used as implemented in Gaussian 09. The potential energy surface was explored using the *ab-initio* molecular dynamics method (ADMP) and a stochastic method (Simulated Annealing) to find starting structures that were optimized with the B3LYP/6-31+G (d) approximation; obtaining 9 stable heterononamers. After reoptimizing those structures including dispersion correction (D3) and a larger base, B3LYP-D3/6-311++G(d,p), the number of stable structures was reduced to 7. The major structural changes were different orientations of the alkyl chains. It was calculated that the most stable heterononamer (Hnon-I) has an isomeric population of 98%. From this structure were designed and optimized homologous structures with only ethanol and with only methanol molecules, as well as a (methanol)8-water structure. Measurements made including geometric, energetic, and topological data. The binding energy (nonamerization) is the difference between the energy of the heterononamer and the sum of the energy of each isolated monomer. In the same way other state functions were calculated (ΔH, ΔS, and ΔG). As an example, the following are the energetic data of Hnon-I: ΔE=-303.68 kcal/mol; ΔH=-339.29 kcal/mol; ΔS=275.32 kcal/K*mol, and ΔG=4.16 kcal/mol. These results imply that the formation of Hnon-I is a highly exothermic and non-spontaneous process. It was found that the cycles formed by O-H---O interactions are fundamental for stabilizing the (hetero) nonamer regardless of their nature. Weaker interactions (C-H---O and H---H) were revealed by means of the molecular graphs calculated through the topological analysis of electron density according to the Quantum Theory of Atoms in Molecules.

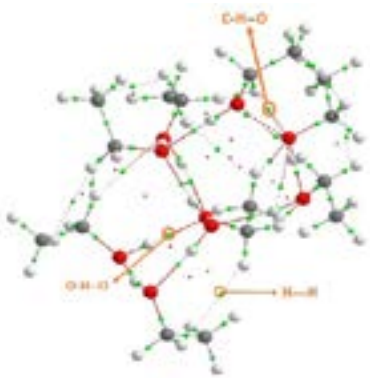

**Figure 1:** *Molecular Graph of Hnon-I: Identification of weak intermolecular interactions by their respective bond critical points enclosed in a circle.*

## Biography

Karen L Zuleta H was born in Bogotá in 1997. She is a student at the Jorge Tadeo Lozano University in the Chemical Engineering program. She is currently doing her research in theoretical and computational chemistry that involve molecular structure, energetic, and binding.