XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

Can molecular hydrogen reduce cytotoxic hydroxyl radical reactivity in aqueous environment? Combined *ab-initio* molecular dynamics and electronic structure investigation.

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Abstract: The reaction between H_2 and OH molecules is demonstrating to be of great importance in medical and biological environments, this surprises researchers because of the non-complexity of the molecules involved in this reaction. The molecule of H_2 is the smallest gas molecule composed of two protons and two electrons, being very stable and reacting only with the oxide radical ion (O^-) [1]. There are several documentations regarding H2, especially in its antioxidant performance. There have been studies of selectivity of H_2 molecule in which cell cultures were induced to an acute oxidative stress and H_2 molecule selectively reduced the more cytotoxic reactive oxygenated species, the hydroxyl radical [1,2,3]. Through researches we could observe that the amount of water in the system was of total influence in the reaction, so the larger the quantity of water, the greater the reactivity [1]. In this project, we performed calculations of Car-Parrinello Molecular Dynamics (CPMD) [4], with several conditions of quantity of OH and H_2 molecules, in vacuum and aqueous solution, in order to map the reaction, however, through the dynamics it was not possible to observe any reaction. We would use the results obtained by dynamics to calculate the reaction rate constant using post-HF and *d*-TST (Deformed Transition State Theory) calculations, but since we did not obtain results, we used a different system from that used in the dynamics. We performed calculations using method MP2-FULL/6-311+G (3df, 2pd) and observed at first something contrary to that reported in researches: with the presence of a water molecule the rate constant decreased, however with the presence of two water molecules we observed an increase of this rate. We observed the rates using the Arrhenius plot. Therefore, we expect that with the addition of more water molecules, this reactivity will continue to increase proportionally. We are performing calculations with other methods to evaluate and

compare the obtained results and to have an average of the system reactional behavior. We hope that with the knowledge of the reaction rates and the reaction behavior of the molecules we can optimize the medical and biological application.

Key-words: Car-Parrinello, antioxidant, *d*-TST.

Support: This work has been supported by CAPES and UEG. Eduardo Vaz would also like to thank PrP/UEG for the assistance.

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