Theoretical investigations on the reactive collisions of the radical (OH) with methanol (CH3OH)

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The reaction of methanol and the hydroxyl radical (OH) is a relevant study topic. In high temperatures, it plays a role in atmospheric combustion, and in low temperatures, it might help explain the presence of CH3O in interstellar clouds. The removal of these compounds inside clouds is done primarily by reactions with hydroxyl radicals. In this work, a theoretical investigation of reactive collisions between hydroxyl radicals and methanol is presented. Calculations of the molecular structure, indicating reaction pathways, are performed. To achieve the task, Density Functional Theory (DFT) and Coupled-Shell Coupled-Cluster (CCSDT) methodologies, from the MOLPRO ab initio package, were employed. In order to evaluate the reliability of obtained energy and structure data, the values from T1 and D1 diagnostics were analyzed. At the minimum and saddle points, T1 diagnostics show very good results, however the D1 values demonstrate an increase, with said increase being indication of non-homogeneity of the electronic structure of the considered molecular systems. It also indicates there is great variability in the orbital rotation parameters of the coupled-cluster wavefunction, i.e., there are problematic zones in the molecule and other zones where the coupled-cluster approach is better suited to be executed. It was observed that occupied orbitals in the studied molecular systems are directly related to system geometry, as well as its energy value. This observation leads us to believe that there are different electronic states at play in this molecular system. The authors thank FAPEMIG in supporting realization of this work.