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| Title: | Does a hydrogen bonded complex with dual contacts show synergism? A matrix isolation infrared and ab-initio study of propargyl alcohol–water complex |
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| Abstract: | When hydrogen bonded complexes are formed with more than one contact, the question arises if these multiple contacts operate synergistically. Propargyl alcohol-H2O complex presents a good case study to address this question, which is discussed in this work. Complexes of propargyl alcohol (PA) and H2O were studied experimentally using matrix isolation infrared spectroscopy, which was supported by quantum chemical computations performed at the M06-2X and MP2 level of theories, using 6-311++G (d,p) and aug-cc-pVDZ basis sets. A 1:1 PA-H2O complex was identified in the experiments and corroborated by our computations, where the PA was in the gauche conformation. This complex, which was a global minimum, showed dual interactions, one of which was an n-σ interaction between the O–H group of PA and the O of H2O, while the second was a H···π contact between the O–H group of H2O and the π system of PA. We explored if the two interactions in the 1:1 complex exhibited synergism. We finally argue that the two interactions showed antagonism rather than synergism. Our computations indicated three other local minima for the 1:1 complexes; though these local minima were not identified in our experiments. Atoms-in-molecules and energy decomposition analysis executed through LMO-EDA were also performed to understand the nature of intermolecular interactions in the PA-H2O complexes. We have also revisited the problem of conformations of PA, with a view to understanding the reasons for gauche conformational preferences in PA. |
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