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| Title: | A Matrix Isolation-FTIR and Ab Initio Study of Ethylene Glycol: Conformations and Hydrogen Bonded Complexes |
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| Abstract: | Ethylene Glycol, a molecule of astrophysical and astrobiological signifi- cance, is the first vicinal diol and has been extensively studied over the years. One of the debates involving ethylene glycol has been the pres- ence/absence of intramolecular hydrogen bonding. Its mixture with water is widely used as an anti-freeze, and the multitude of positions available for water to orient itself around the ethylene glycol has motivated this study. Matrix Isolation technique coupled with Infrared spectroscopy has been used to study the conformations and water complexes of ethylene glycol in nitrogen and argon matrices. Three conformations are seen in the ni- trogen matrix, while two are seen in the argon matrix. In the nitrogen matrix, three complexes corresponding to the two lower energy conformers are observed. The conformational analysis of ethylene glycol has been computationally studied using various levels of theories. The optimised structures for the (1:1) water complexes corresponding to the three lowest energy confor- mations are also presented. Along with providing the analysis of orbital interactions for these complexes to give the chemical bonding picture, the strengths of the hydrogen bonding interactions are also calculated.<br>Ethylene Glycol, a molecule of astrophysical and astrobiological significance, is the first vicinal diol and has been extensively studied over the years. One of the debates involving ethylene glycol has been the presence/absence of intramolecular hydrogen bonding. Its mixture with water is widely used as an anti-freeze, and the multitude of positions available for water to orient itself around the ethylene glycol has motivated this study. Matrix Isolation technique coupled with Infrared spectroscopy has been used to study the conformations and water complexes of ethylene glycol in nitrogen and argon matrices. Three conformations are seen in the nitrogen matrix, while two are seen in the argon matrix. In the nitrogen matrix, three complexes corresponding to the two lower energy conformers are observed. The conformational analysis of ethylene glycol has been computationally studied using various levels of theories. The optimised structures for the (1:1) water complexes corresponding to the three lowest energy conformations are also presented. Along with providing the analysis of orbital interactions for these complexes to give the chemical bonding picture, the strengths of the hydrogen bonding interactions are also calculated. |
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