CONFORMATIONAL ISOMERIZATION BARRIERS AND DYNAMICS OF PHENOL-ETHANOLAMINE CLUSTERS

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Stimulated emission pumping (SEP)-population transfer spectroscopy has been used to place upper and lower bounds to the barrier heights for conformational isomerization between two of the three conformational minima of phenol-ethanolamine van der Waals complexes. These two minima differ in the point of attachment of the phenol OH hydrogen bond to the oxygen atom of ethanolamine. The thresholds for X $\rightarrow$ Y and Y $\rightarrow$ X isomerization are combined to determine the relative energies of the X and Y minima. Comparison of experimental data to *ab initio* computed barriers will be made, leading to the identification of the low-energy isomerization pathways linking the minima. Despite adequate sensitivity, isomerization involving the third minima, in which phenol acts as H-bond donor to the NH_2 group and as acceptor to the ethanolamine OH, is not observed. This cyclic solvent configuration exhibits a fluorescence lifetime 3 times shorter than the other two conformations of the complex, with red-shifted fluorescence emission. The shortened fluorescence lifetime and red-shifted emission were attributed to excited state H-atom transfer as a non-radiative energy transfer process.