Significance / Novelty.

In the present work we have undertaken the computational study of the H-bonded complexes of methyl sulfinyl radical with one molecules of sulfuric acid and their subsequent hydration with one or two water molecules. We aim to investigate and characterize the nature of the interactions that holds these complexes together, to report accurate results regarding binding energies for their formation and to provide essential spectroscopic information that would aid in their experimental characterization in the laboratory as well as in the field measurements. The primary focus is devoted to predict the influence of H-bonding on the IR spectra of the H-bonded OH stretching vibrations in the complexes. The vertical excited state energies of the complexes are calculated to determinate to what extent the complexation might influence the electronic spectra of radicals within the acid and water complexes. The CH_3SO-sulfuric acid-water complexes and their hydration have not, to best of our knowledge, been reported before, either experimentally or theoretically. Due to their role in the new particle formations in the troposphere this type of studies are highly desirable. High-level density functional and ab initio calculations represent a powerful tool for gaining insight into nucleation mechanism at molecular level, for instance, they are able to describe the very first step of particle formation in the atmosphere.