



## **HNO<sub>3</sub>/HCl/H<sub>2</sub>O CLUSTERS: PREDICTION OF SPECTRA**

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Water, nitric acid and hydrogen chloride take part in several atmospheric processes, among which that of the complex reactions related to ozone depletion in polar stratospheric clouds (PSC). IR spectroscopy is one of the main techniques used to study the atmospheric properties.

We have carried out theoretical calculations at the B3LYP/aug-cc-pVQZ level to predict the IR and MW spectra of ternary clusters of water, hydrogen chloride and nitric acid. Fifteen of these clusters are expected to be thermodynamically stable species, and three would form spontaneously at stratospherically relevant temperatures.

The main IR spectral features of these clusters can be analyzed in terms of the different hydrogen bonding characteristics of the aggregates. Based on a calculation of the Gibbs free-energy of formation of the clusters from their monomers, we have evaluated their population distribution at atmospherically relevant temperatures, from which we predict the IR spectra of the composed mixture. The variations of specific spectral features with temperature are significant, and could be used to detect the possible existence of these clusters, as well as to provide an indication of the temperature of the corresponding atmospheric sample.

We also discuss the formation of these clusters in laboratory experiments and their possible identification based on their infrared and microwave spectral properties.

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