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Spectroscopic Properties of Aerosols and their Microscopic Origin

RUTH SIGNORELL, University of British Columbia

Large molecular aggregates with sizes ranging from less than nanometers up to microns play an important role in atmospheric processes, as components of the interstellar medium, and as drug delivery systems in medicine. The vibrational dynamics of these particles can be strongly influenced by intrinsic particle properties such as size, shape, or surface area. These phenomena are discussed here for several pure and composite ice particles which consist of CO₂, N₂O, NH₃, SO₂, their isotopomers, and different carbohydrates. The aerosol are generated in collisional cooling cells, by supersonic expansions, and by rapid expansion of supercritical solutions [1]. The vibrational dynamics is studied in situ with a rapid scan Fourier transform infrared spectrometer. We demonstrate that only the combination of experiments with microscopic models leads to a comprehensive understanding of the various features observed in the infrared spectra. The corresponding molecular model (exciton model [1,2]) allows us not only to calculate spectra for large molecular aggregates, but also to derive propensity rules for the occurrence of characteristic effects in infrared spectra of particles.

[1] R. Signorell, *Mol. Phys.* **101**, 3385, (2003).

[2] R. Disselkamp and G. E. Ewing, *J. Chem. Soc. Faraday Trans.* **86**, 2369, (1990).