



Vibrational spectra of nitric acid hydrates

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Nitric acid hydrates are important constituents of solid PSC and Cirrus cloud particles. Due to the phase diagram only hexagonal ice and nitric acid trihydrate have a reasonable thermodynamic stability and are commonly observed in the stratosphere. Besides, also a number of metastable modifications might exist: α -NAD, β -NAD, α -NAT, NAP and cubic ice. The existence of these metastable compounds remains uncertain and has not been proven yet.

In the laboratory we have developed a model procedure in order to prepare and investigate all hydrates as pure phases. The investigation methods are X-ray diffraction [1], [2], FTIR spectroscopy [3] and Raman spectroscopy [4]. The aim is to verify the phase composition by diffraction and collect the spectroscopic data of the respective phases, which are needed for interpretation of field measurements and aerosol chamber experiments.

Particular interest has been directed towards the modifications of NAD, which have been discriminated for the first time by spectroscopic methods. Beside the mid-IR region, where normal vibrations have been assigned, we have also focused on the low-frequency region below 200 cm^{-1} where phonon bands are observed by Raman spectroscopy. These intermolecular vibrations are closely connected to the symmetry and structure of the unit cell of a hydrate crystal. Thus, a distinction between the phases becomes easily accessible.

[1] H. Tizek, E. Knözinger, H. Grothe, PCCP 4 (2002), 5128.

[2] H. Tizek, E. Knözinger, H. Grothe, PCCP 6 (2004), 972.

[3] H. Grothe, C.E. Lund Myhre, H. Tizek, Vibr. Spectr. 34 (2004), 55.

[4] H. Grothe, C.E. Lund Myhre, C.J. Nielsen, J. Phys. Chem. A 110 (2006) 171.