Title: Mass spectrometric and optical spectroscopy studies of clusters and nanoparticles in molecular beams

Author: Kamila Moriová

Institute: Institute of Physics of Charles University

Supervisor: doc. Mgr. Michal Fárník, Ph.D., DSc., J. Heyrovský Institute of Physical Chemistry of the CAS

Consultant: RNDr. Václav Profant, Ph.D., Institute of Physics of Charles University

Abstract: Condensation of ices on the surface of dust grains with activation of these ices by cosmic rays in interstellar medium can lead to formation of complex chemical species. In the present work we primarily examine ammonia clusters, which represent a model system of ice particles. Large ammonia clusters were prepared in molecular beams and pass through a pickup chamber in which methanol molecules were captured. After electron ionization of \((\text{NH}_3)_N(\text{CH}_3\text{OH})_M\) clusters, a mass spectrum of ionic fragments was obtained in which fragments with methanol \((\text{NH}_3)_n(\text{CH}_3\text{OH})_m\text{H}^+\) predominated over the pure ammonia fragments \((\text{NH}_3)_n\text{H}^+\): at least one methanol molecule was present in 75% fragments. This is in disproportion with the composition of the original neutral precursors, which contain less than 4% of methanol. Based on the measurement results, we suggest that ammonia is ionized in the first place resulting in the \(\text{NH}_4^+\) ion core solvated with either ammonia or methanol molecules, which have a strong propensity for sticking to the fragment ion. The principle of ionization mechanism and ion-molecular reactions was investigated in experiments with partially deuterated methanol. The measurements did not show any evidence for the proton transfer from the methyl group of methanol. Proton transfer from the hydroxyl group cannot be excluded unambiguously.

Keywords: mass spectrometry, molecular beams, electron ionization, clusters