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A preliminary view on adsorption of organics on ice at temperatures close to melting point

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Ice and snow play active roles in the water cycle, the energy budget of the Earth, and environmental chemistry in the atmosphere and cryosphere. The uptake of trace gases from the atmosphere may induce changes in the structure of the surface layer of ice crystals and has important consequences for atmospheric chemistry and the climate system. However, a molecular-level understanding of trace gas adsorption on ice is still missing, and also little is known about the impurity-induced ice-surface disorder in the context of environmental relevance.

It is a general challenge to apply highly sensitive experimental approaches to ambient air conditions, e.g. studies of volatile surfaces, because of the strict requirements of vacuum experimental conditions. In this study, we employed synchrotron-based X-ray Photoelectron Spectroscopy (XPS) and partial electron yield Near Edge X-ray Absorption Fine Structure (NEXAFS) in a state-of-the-art Near-Ambient Pressure Photoelectron (NAPP) spectroscopy end station. The NAPP enables to utilize the surface sensitive experimental methods, XPS and NEXAFS with electron detection, on volatile surfaces, i.e. ice at temperatures approaching zero degree Celsius. XPS and NEXAFS provide unique information of hydrogen bonding network, surface concentration of organic adsorbates, depth profile of dopants in the ice, and acid-base dissociation on the surfaces. For instance, a few carboxylic acids, e.g. acetic acid and formic acid, have been recently studied by XPS and NEXAFS in NAPP.

Amines are a group of nitrogen-containing basic organics with atmospheric relevance. Only few studies have been focused on amines, and atmospheric models rarely take account of them due to the limitation of knowledge. Several amines have been found to play active roles in the processes of aerosol formation, e.g. dimethylamine (DMA), trimethylamine (TMA) and 1-propanamine. In this study, we will focus on one of these three amines after pre-tests, and perform core-level spectroscopies to reveal the behaviour of adsorption and dissociation on ice. Additionally, pure ice and amine doped ice will be compared for their surface structure change at different temperatures, which will indicate the differences of surface disordering caused by different factors. For instance, we will have a chance to know better if impurities will cause local disordering, i.e. forming hydration shell, which challenges the traditional picture of a homogenous disordered doped ice surface. The findings of this study could not only improve our understanding of how acidic organics adsorb to ice, and of their chemical properties on ice, but also have potentials to know better the behaviour of pure ice at temperatures approaching to the melting point.