Geophysical Research Abstracts,
Vol. 11, EGU2009-1057, 2009
EGU General Assembly 2009

Atmospheric ice particles on the molecular level - laboratory experiments and computer simulations

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This talk will review recent laboratory studies and computer simulations related to the formation, properties and heterogeneous chemistry of atmospheric ice particles. Molecular beam techniques have been used to provide molecular level information about molecule-ice interactions, and to probe structural changes of ice surfaces. The saturated water vapour pressure above ice at tropospheric and stratospheric temperatures is significant, which makes it difficult to probe surface processes using ions, electrons, atoms or molecules. This problem is partially overcome in the present studies where an elevated water vapour pressure outside the ice surface made it possible to follow gas-ice interactions at temperatures up to 200 K under steady state conditions, i.e. no net evaporation or condensation.

The surface of water ice was probed by elastic helium scattering, which showed that the properties of the top-most molecular layer on ice changes around 180 K. This change is a first sign of increased mobility of water molecules at the surface, which precedes the formation of a quasi-liquid layer at higher temperatures. The fact that the changes occur around 180 K indicates that water ice will have disordered surfaces under the conditions prevailing in the lower atmosphere on earth. The experimental method has also been used to study heterogeneous ice nucleation by deposition freezing and examples from these studies will be described. Furthermore, the uptake of trace gases and heterogeneous chemistry of relevance for the upper troposphere and lower stratosphere have been studied with similar methods, and results for nitrogen oxides and chlorine-containing molecules, including HCl and HNO3, will be presented. In parallel, computer simulations were used to study the mechanisms in operation and also to provide detailed information about the dynamics of ice particle-particle collisions.

Future prospects for the application of molecular beam techniques to ice and water studies of atmospheric relevance will be discussed.