Geophysical Research Abstracts,
Vol. 11, EGU2009-10553-1, 2009
EGU General Assembly 2009
© Author(s) 2009

Simulation of the interaction of acetone with ice: (0001) surface, bulk ice and small-angle grain boundaries

S. M. Hammer (1), R. Panisch (2), M. Kobus (3), J. Glinnemann (1), and M. U. Schmidt (1)

(1) Goethe University, Institute of Inorganic and Analytical Chemistry, Frankfurt am Main, Germany (hammer@chemie.uni-frankfurt.de), (2) Carl von Ossietzky University Oldenburg, Institute of Pure and Applied Chemistry, Oldenburg, Germany, (3) Goethe University, Institute of Physical and Theoretical Chemistry, Frankfurt am Main, Germany

Local structures and energies are calculated for the interactions of acetone with ice I_h by force-field and *ab-initio* methods.

Three interaction sites are investigated:

1) (0001) surface of ice

2) ice bulk (with the acetone substituting one or more water molecules as point defect)

3) small-angle grain boundaries in ice (2D-lattice defects)

Ice I_h is the stable ice polymorph at atmospheric conditions.[1] When ice (snow/hail/graupel) begins to form in the troposphere, volatile organic compounds will be adsorbed at the surface or incorporated into the crystals. Acetone $(CH_3)_2CO$ is one of the most prominent organic pollutants in the atmosphere.

For the force-field calculations a modified Dreiding force field[2] was used.

Results[3]

1) An acetone molecule adsorbed on the (0001) surface of ice forms two hydrogen bonds between the CO group and two dangling O-H bonds ($i.e.$ bonds which stick out from the surface) of two water molecules. The calculated adsorption enthalpy corresponds well with experimentally determined values. This geometry was confirmed by *ab-initio* calculations.

2) In bulk ice, the acetone molecule replaces only one water molecule, and distorts the surrounding ice structure.

3) The position of an acetone molecule at a small-angle grain boundary or at a similar lattice defect is energetically more favourable than incorporation in bulk ice.

[1] V. F. Petrenko and R. W. Whitworth, *Physics of Ice*, Oxford University Press Inc., New York, 1999.

[2] S. L. Mayo, B. D. Olafson, W. A. Goddard III, *J. Phys. Chem.* **1990**, 94, 8897-8909.

[3] S. M. Hammer, R. Panisch, M. Kobus, J. Glinnemann, M. U. Schmidt, *CrystEngComm* **2009**, accepted.