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Adsorption of Acetone on Ice at Temperatures between 190 and 220 K: Thermodynamic Data and Kinetic Model Simulation

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The kinetics and thermodynamics of adsorption of acetone on ice surfaces were measured in a temperature range between 190 and 220 K using a Coated Wall Flow Tube (CWFT) equipped with mass spectrometric detection. Ice surfaces of variable thicknesses (10-300 μm) were prepared by water vapour condensation.

The results show that the adsorption of acetone on ice surfaces follows Langmuir behaviour. The adsorption capacities, however, decrease with increasing age of the ice surface with the extent of this decrease being dependent on temperature. In agreement with quantum-mechanical calculations [1] and FTIR spectroscopic investigations [2] the observed adsorption behaviour on a fresh ice surface indicates that two different active centers with adsorption enthalpies of ΔH_{ads} = -48 $\pm$ 5 kJ/mol and ΔH_{ads} = -30 $\pm$ 6 kJ/mol exist, which can be assigned to amorphous and crystalline regions, respectively. The temperature-dependent decrease of the adsorption capacity of the surface during ageing can be attributed to the decrease of defects at the surface, paralleled by a phase change from the amorphous to the crystalline structure. The maximum surface coverage increases from approximately 5*10^{14} molecules/cm^2 for a thickness of about 10 μm to 2*10^{15} molecules/cm^2 for a thickness of about 300 μm. Kinetic data of the individual adsorption and desorption processes at different sites have been determined using a kinetic model simulation developed for reversible gas adsorption in CWFT-reactors [3].

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