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A study of sulfur dioxide adsorption on an ice Ih surface

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FTIR spectroscopy and *ab initio* calculations have been applied to study the processes of SO_2 adsorption and further oxidation reactions on water ice surfaces. These studies provide valuable information about the role of ice clouds (e.g. cirrus) for the atmospheric oxidation of SO_2 molecules. In order to explain the observed features in the FTIR spectra and flow depositon experiments, *ab initio* cluster calculations of various surface and crystal models of ice were performed using the density functional theory at the B3LYP/6-31++G(d,p) level. The surface models used in the study consisted of up to 29 water molecules arranged in agreement with the "ice rules" and modelling the different sites at the basal and side planes of ice Ih: terminal O (tO) and terminal H (tH) atoms, tO-tO, tO-tH, and tH-tH pairs. Various coordination modes of SO_2forming hydrogen-bonded adsorption complexes at the surface or inside the ice I$h$crystal were considered: (i) adsorption on the basal and side planes, (ii) inclusion into the interstitial space of the ice crystal structure, (iii) incorporation into the crystalline network. In order to describe the various adsorption modes at the ice surface, the new method was applied which was especially developed for the modelling of orientationally disordered clusters, crystals and surfaces. A comparison has been made for the adsorption energies of SO_2 with experimental data available from different literature sources. On this basis thermodynamic parameters and IR spectral properties of the adsorbed species were estimated.