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Molecular dynamics simulations of acetic acid adsorbed on ice at tropospheric temperatures.

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In this work, we have investigated the adsorption of acetic acid molecules on ice at tropospheric temperatures [193 – 223 K]. The simulations have been done as a function of the adsorbate coverage, up to the completion of one monolayer above the ice surface. The results of the simulations show that the interaction between acetic acid molecules and the ice surface is governed by the formation of hydrogen bonds with water molecules. At high coverage, the adsorption process is also influenced by the formation of lateral hydrogen bonds within the adsorbate. The calculated saturation coverage for acetic acid on ice is equal to about 3.7×10^{14} molecules/cm^2, and the corresponding mean adsorption energy per molecule is equal to -69.5 kJ/mol at 193 K. The results of these simulations compare fairly well with available experimental data obtained from coated wall-flow tube experiments, especially in terms of adsorption energy and saturation coverage. Moreover, the simulations indicate that the interaction with the ice surface is strong enough to break the acetic acid dimers that exist in the gas phase, and leads rather to the stabilization of acetic acid monomers on ice.