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Adsorption of halogenated methane derivatives at the ice surface under tropospheric conditions, as seen from Grand Canonical Monte Carlo simulations

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The adsorption of all the fluorinated and chlorinated methane derivatives at the surface of Ih ice is studied by grand canonical Monte Carlo simulations at 200 K.
The adsorption isotherms are simulated and their shape is discussed in terms of the interplay of adhesive and cohesive interactions. It is found that in cases when the adhesive interaction is
clearly the stronger one, multilayer adsorption occurs; when the cohesive interaction is the dominant one, no considerable
adsorption is observed, while in cases when the two interactions are of roughly the same strength, the formation of a saturated monolayer occurs. The isotherms exhibit the Langmuir shape, at least up to the
pressures where multilayer adsorption starts to occur, given that the cohesion acting between the adsorbate molecules is only moderately strong. Too strong cohesion, on the other hand, leads to the deviation of the isotherm from the Langmuir shape. While the strength of cohesion depends on the properties of the adsorbate molecules, that of adhesion is determined by hydrogen bond formation between the adsorbed molecules and the ice surface. Our results also reveal that the surface
orientation of all these adsorbed molecules is such that at least one of
their halogen atoms is exposed to the vapour phase, which makes it
easily accessible for reactions with gas phase species, and also easily
releasable in photodissociation processes.

Significance statement

First full characterization of the adsorption process of halogenated methane derivatives on ice, by means of Monte Carlo simulations in the Grand Canonical Ensemble.

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