

## Computer simulation investigation of the adsorption of acetamide under atmospheric and interstellar conditions

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### ABSTRACT

Acetamide is not only released into the atmosphere from natural sources, but its large-scale industrial use also results in its atmospheric emission. The main atmospheric sink of acetamide is its oxidation, however, other atmospheric fates are also plausible. In wet deposition, acetamide can be captured by ice grains through adsorption. Thus, we investigated the adsorption of acetamide at the surface of crystalline ( $I_h$ ) and low density amorphous (LDA) ices by performing a set of grand canonical Monte Carlo simulations at the tropospheric temperature of 200 K. Besides calculating the adsorption isotherms, we also characterised the energetics of the adsorption and the orientational preferences of the first layer molecules. We demonstrated that at low enough surface concentrations, the adsorbed acetamide molecules prefer to lay parallel with the ice surface. With increasing surface coverage, acetamide molecules preferentially stay perpendicular to the surface, pointing by the  $\text{CH}_3$  group straight away from the ice phase, typically forming 2 H-bonds with each other and 2 with the surface waters. Finally, after the appearance of outer layer acetamide molecules, first layer molecules prefer to form 3 H-bonds with their acetamide neighbours and only 1 with the surface waters.

As acetamide has been detected in a relatively large amount in space as well, we extended our study by performing grand canonical Monte Carlo simulations at 50 and 100 K on LDA ice, which are more characteristic of typical domains of the interstellar medium. We found that the relative importance of the acetamide–acetamide H-bonds with respect to the acetamide–water ones increases with decreasing temperature. As a result of it, the saturated monolayer, which is stable in a broad range of chemical potentials at 200 K, shrinks with decreasing temperature, and, eventually, vanishes at 50 K, while multilayer adsorption becomes more and more pronounced at the lower temperatures. Furthermore, our results suggest that non-negligible acetamide adsorption might occur on LDA surfaces at low enough temperature (i.e., 50 K and below), thus, the interstellar formation of peptide chains through acetamide molecules might well be a plausible process in the cold domains of the interstellar medium; however, it is rather unlikely in the higher temperature domains.