

Adsorption of methylamine on amorphous ice under interstellar conditions. A Grand Canonical Monte Carlo simulation study

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Methylamine is a potential precursor of the amino acid glycine, as its reaction with CO₂, occurring at the surface of water or ice, results in glycine. It is thus widely assumed that the formation of glycine in the period of chemical evolution (i.e., before the occurrence of the proteins and nucleic acids in the prebiotic Earth) occurred, at least partly, through this reaction. On the other hand, both methylamine and CO₂ are also present in the interstellar medium, and glycine was detected at the surface of several meteorites when arriving to the Earth. *Ab initio* calculations showed that aqueous surfaces catalyze this reaction, and the production rate is increased at lower temperatures. The main hindrance of the possibility of this reaction occurring in the space is the extremely low concentration of the reactants in the interstellar medium. To investigate the possibility whether this low concentration can be locally substantially increased, we investigate here the adsorption of methylamine at the surface of amorphous ice, known to be in abundance in the space, at low temperatures ranging from 20 K to 200 K, by computer simulation methods.

Our results show that methylamine is strongly adsorbed at the surface of amorphous ice, this adsorption can involve several molecular layers, and, as is expected, it is enhanced at lower temperature. The chemical potential corresponding to the point of condensation increases linearly with decreasing temperature, indicating that the corresponding (molar) entropy is temperature independent. It is also found that, contrary to crystalline ice, methylamine is also dissolved in a small, yet detectable concentration in the bulk phase of amorphous ice. Apart from the contribution of the dissolved molecules (which cannot be distinguished *on the fly* from the adsorbed ones), the obtained isotherms can be reasonably well fitted by the Langmuir isotherm. The steepness of the fitted Langmuir function increases extremely rapidly with decreasing temperature, resulting in a considerable surface density already at the very low relative pressure range of 10⁻²⁵-10⁻³⁰ at 20 K. This finding confirms the possibility that considerable methylamine adsorption at icy surfaces might well occur in the interstellar medium.

We have also analyzed the surface orientation and binding energy distribution of the first layer methylamine molecules. Our results show that these molecules can form up to three hydrogen bonds with the surface waters, and the average binding energy of an adsorbed methylamine molecule at very low surface concentration is only slightly, by about 5 kJ/mol smaller than that of the dissolved molecules.