

Investigation of Methylamine at Aqueous Surfaces by Computer Simulation Methods

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Methylamine is already known for its relative atmospherical and interstellar abundance among amines, therefore many theories assume a special role of it in the prebiotic evolution as well as in several reactions included in the nitrogen cycle of the Earth. According to *ab initio* calculations and experiments, aqueous surfaces have a catalytic effect on these reactions through their interaction with methylamine. For examination of the behaviour of methylamine at icy surfaces and at the liquid-vapour interface of water-methylamine mixtures computer simulations were performed.

Related to the panspermia hypothesis the adsorption equilibrium of methylamine was investigated on the surface of amorphous ice, which is characteristic to the interstellar medium, by grand canonical Monte Carlo simulation method at five different temperatures ranging from 200 K to 20 K. We demonstrated the strong tendency of methylamine molecules for being adsorbed at the surface of amorphous ice, including their ability for multilayer adsorption. Our analyses revealed that the methylamine prefers to be in all the orientations where the carbon-nitrogen bond axis lays parallel with the macroscopic ice surface, and also that at low chemical potential values the methylamine tends to form up three hydrogen bonds with the surface water molecules of the amorphous ice.

The liquid-vapour interface of aqueous methylamine solutions of several different, finite concentrations was also investigated by molecular dynamics simulation method. Our results indicated that methylamine molecules show a tendency to be accumulated in the first molecular layer, however, they do not show considerable self-association at the surface of their aqueous solutions. Surface methylamine molecules strongly prefer the alignment in which the apolar CH₃ group points straight to the vapour phase. The presence of the methylamine accelerates the exchange of methylamine and water molecules between the surface layer and the bulk phase, furthermore, methylamine molecules slow down the lateral diffusion of each other and immobilise the water molecules within the surface layer.

As a consequence, we have seen that methylamine could play indeed a special role in the prebiotic evolution as it is described in the panspermia hypothesis, and based on our results, it is also possible that the methylamine might participate in atmospherical reactions.