

P053

Adsorption of Methylamine on Amorphous Ice under Interstellar Conditions. A Grand Canonical Monte Carlo Study

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Introduction

Panspermia hypothesis

- formation of biogenic molecules in the interstellar medium
- travelling to the prebiotic Earth at the surface of meteorites

Formation of glycine under interstellar conditions
 $\text{CO}_2 + 2 \text{CH}_3\text{NH}_2 \rightarrow [\text{CH}_3\text{NH}_2]^+[\text{NH}_2\text{CH}_2\text{COO}]^-$ under UV radiation, at low T

Methylamine

- precursor of glycine
- high reactivity at icy surfaces
- formation on interstellar amorphous ice

CO_2

- detected in the interstellar medium

Amorphous ice

- covers the surface of meteorites

However, does methylamine stay adsorbed at the surface of amorphous ice?



Reactants

Glycine formation at icy surfaces

Glycine was detected at the surface of meteorites

Methodology

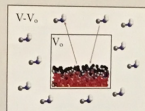
The adsorption capacity of methylamine on amorphous ice has been studied by grand canonical (T, V, μ) Monte Carlo method at five various temperatures (200, 150, 100, 50 and 20 K).

Monte Carlo steps include:

- by 50% probability methylamine insertion or removal (25-25%)
- by 50% probability translation and rotation (not more than 25 Å and 15°)

Computational details

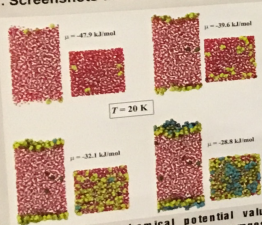
- TIP3P water model¹
- Methylamine model by Impey et al.²
- 2880 water molecules
- Approximately $10^3 - 10^4$ MC steps in each simulation
- Box parameters: X=100 Å, Y=38.891 Å and Z=35.828 Å
- At each T selected μ values for further analysis (5000-5000 configuration)



The molecular layers were distinguished by ITIM analysis³ from each other

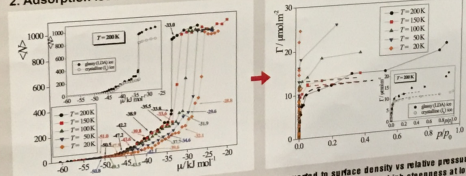
Results and consequences

1. Screenshots at 20K

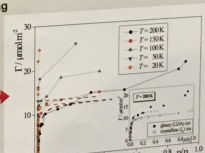


- Four selected chemical potential values corresponding to different surface coverages at the 20K (it is a characteristic temperature of the interstellar medium)
- Multilayer adsorption at higher chemical potential values
- Dissolved methylamine in the bulk ice phase

2. Adsorption isotherms and Langmuir fitting

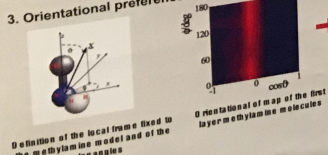


- Isotherms shifted to higher chemical potential values with decreasing temperature
- No plateau: multilayer adsorption before saturated monolayer
- Higher adsorption capacity on amorphous ice than on crystalline ice due to the corrugated ice surface



4. Energy distribution

- Energy of a hydrogen bond: 20-25 kJ/mol
- Peaks corresponding 3, 2, 1 and 0 hydrogen bonds
- The contribution of the methylamine-ice interaction decreases with increasing μ (the number of the H bonds increases)
- The lateral contribution increases
- The total binding energy unchanged



- Preferable alignment at cos θ = 0 → CH₃-H bond lays parallel to the surface
- Along φ there is no preference, so methylamine could be in many different orientations

In the orientational map of the surface water molecules of the amorphous ice there isn't any preferences neither → the role of hydrogen bonds

Summary

Methylamine has a strong ability to be adsorbed at the surface of amorphous ice under interstellar conditions (at a low but not too low chemical potential). The adsorption contains several molecular layers, moreover considerable methylamine concentration could form up three hydrogen bonds with the surface water at low chemical potential.