
Adsorption selectivity on interstellar surfaces: computational experiments. Local versus global approach.

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Résumé

Astrophysical/Computational Context

It is now well admitted that, to account for the diversity of complex organic molecules (COMs) observed in the Interstellar Medium (ISM), solid-gas reactions and chemical processes involving adsorbed partners have to be considered. The equilibrium between the molecules on the surface and those in the gas phase will depend on the adsorption energies *critically*. Consequently, the physical process of surface adsorption/desorption is now considered among major processes in astrochemistry.

Quantitative results for adsorption energies are hard to get, experimentally as well as theoretically, taking into account that both, nature of the surface and nature of the molecule intervene in their own way. To this end we rely *on numerical simulations based on the methods of quantum chemistry, namely Density Functional Theory (DFT)* that proved efficient in the *periodic approach* to this category of phenomena.

Selective adsorption phenomenon

Adsorption has definitively to be taken into account in the astrochemical modeling. More precisely, we consider here selective adsorption as to interpret isomers abundances and as a possible process for enantiomeric enhancement.

In cold molecular clouds, the grains are most probably covered with ice. As the temperature increases, the ice should vaporize, the less bound molecules being first released in the gas phase, followed by H₂O, revealing the bare grain underneath on which molecules may re-adsorb and be ready for a new kind of reactivity. Such a mechanism of recycling, implying *adsorption on different types of interstellar surfaces* could be a major process in astrochemistry and have a direct impact on the relative abundances of isomers observed in the gas phase.

Two enantiomers have identical internal energies. When adsorbed on a same chiral surface, the complexes obtained are no longer enantiomers, but diastereoisomers. These diastereoisomers do not have the same energy. Assuming that we have a chiral

*Intervenant

interstellar surface at hand, we can consider the possibility to *adsorb selectively one of the two enantiomers* and thus engage a process of enantiomeric enhancement.

Results

We present several examples of increasing complexity, mixing adsorbates going from atoms to prebiotic molecules, and surfaces as graphene, water ices and silica, to end with the enantio-selective adsorption of R/S lactic acid and alanine on a chiral active α -quartz surface. Adsorption shows strong dependence with the site for complex molecules adsorbing on complex surfaces and a statistical treatment giving a global response of the surface is proposed for such cases.

Conclusion

Adsorption may depend strongly of the site, especially for complex surfaces and complex molecules. The question of the suitability of a statistic treatment could arise according the degree of complexity, the coverage of the surface and the precision needed. Also, the astrophysical meaning of each solution, local versus global, is open to discussion.