A New Approach to Compute the Accurate Binding Energy Distribution of Molecules at Ice Interstellar Grain Models: the Case of NH_3

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In the denser ($\geq 10^4$ cm^{-3}) and colder ($\leq$20 K) regions of the interstellar medium (ISM), sub-micron sized dust grains are covered by several layers of H_2O-dominated ices [1]. The composition and thickness of these ices is governed by whether molecules and atoms remain glued to the grain surfaces or not and whether they can move on the surfaces and scan them, so to meet other species and react. On the other hand, in warmer regions, these interstellar ices can (partially) sublimate and enriched the gas of its components. The ice-gas interaction is, therefore, a hugely important process that determines the chemical composition of the ISM. The basic quantity that rules all these processes is the binding energy (BE) of the species to the interstellar ice surface. It is thus not an exaggeration to affirm that the BE of interstellar atoms and molecules is a small quantity with a huge impact. So far, with very few exceptions, astrochemical models have assumed single values for each species BE. In this work, we present a new and robust computational strategy to evaluate BEs by theoretical computations on a novel amorphous solid water (ASW) cluster [2]. This cluster exhibits a large number of adsorption sites where NH_3 (our test molecules) can be adsorbed. The BEs are computed through the ONIOM [3] approach using a QM:QM layer envisaging xTB-GFN2 [4] as the low method and DLNPO-CCSD(T) [5] as the high level method. The generality of xTB-GFN2 as a low-level method allows to treat a large variety of interstellar species, at variance with the adoption of *ad hoc* force fields as currently done in the literature. As a first study and astrochemically important case, we applied this new methodology, to derive the BE distribution of ammonia, computed on about 160 different adsorptions shown in the right figure. Machine learning clustering analysis is performed and further the two clusters found were fitted by Maxwell-Boltzmann distributions, which reflect the different nature of the possible bonds of NH_3 on ASW. Particularly important is the low-energy end of the BE distribution, which has an unexpected impact on some astrochemical situations, like protoplanetary disks.

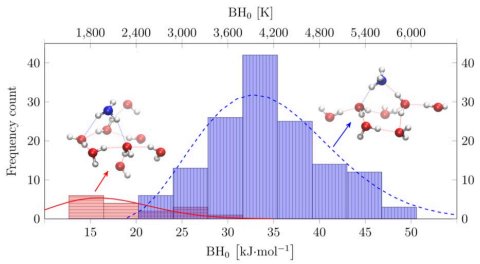

Figure 1: *NH_3 ZPE corrected BE Distribution*

References

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