Insights into the Third-Body Role of Interstellar Water Ices Mantles in Formamide Formation Route

B. Martínez-Bachs,[1] G. Pareras,[1] J. Enrique-Romero,[2] and A. Rimola[1]

[1]*Universitat Autònoma de Barcelona, Departament de Química, 08193 Bellaterra, Spain*
[2]*Leiden Institute of Chemistry, Leiden, University, Leiden 2300 RA, The Netherlands*

Ice mantles covering dust particles provide a solid-state support for chemical reactions in the Interstellar Medium. Such water ice surfaces can act as third bodies by absorbing the energy released by surface reactions [1]. Indeed, the ability of ice mantles to absorb the energy released by surface reactions is a crucial factor that will determine the fate of the newly formed species. These species can either remain adsorbed on the ices or be desorbed and ejected into the gas phase, as is commonly assumed by astrochemical models [2-4]. In this contribution, we analyze the third-body role of water ice mantles for a particular reaction: the radical-radical coupling between NH_2 and HCO leading to the formation of formamide. This mechanism presents a low energy barrier and is largely exothermic [5]. Its potential energy surface has been characterized on an amorphous water ice model using static quantum chemical methods. Ab initio molecular dynamics simulations have been performed to elucidate how the nascent reaction energy is dissipated through the amorphous water ice model. Results indicate that the energy release by the reaction is effectively absorbed and dissipated by water ices, and therefore, the energy reaming on the newly formed formamide is not large enough to cause its ejection into the gas-phase.

References

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