Growth of unsaturated, cyclic, and polycyclic aromatic hydrocarbons: Reactions under the conditions of the interstellar medium

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Hydrocarbons, in particular polycyclic aromatic hydrocarbons (PAHs), have been long discussed to be carriers of many interstellar infrared (IR) emission bands and ultraviolet (UV) absorption features. Yet, the origin of PAHs in dense phases of the interstellar medium, such as molecular clouds, remains unclear.

In this work, growth mechanisms based on ion-molecule reaction between cationic PAHs / hydrocarbons and methyne (CH) were investigated. The reaction type and the precursor were derived and selected from known chemical and physical properties of the ISM. The chemical reactions were characterised by calculating reaction parameters such as branching ratios and capture rate coefficients, minimum reaction paths, reaction enthalpies, thermal equilibrium constants, and microcanonic isomerisation and radiative deactivation rate coefficients. In order to cope with the variety of reaction parameters, a hierarchic workflow scheme was set up. It consisted of a potential energy surface sampling near the reaction centre by molecular dynamics simulations (using tight-binding based DFT), followed by a minimum energy path search (at DFT level of theory) of statistically selected reaction channel trajectories, and reoptimisation of stationary points (at post-Hartree-Fock level of theory).

Results on CH based hydrocarbon growth showed the transition from non-cyclic hydrocarbons to cyclic and aromatic structures, and from cyclic to polycyclic aromatic hydrocarbons. Additionally, the reactive collisions between hydrocarbons and CH were found to produce sufficient energy for isomerisation and fragmentation processes even at ultra low temperatures. In all, the results indicate that methyne might be a proper precursor for the formation of large interstellar PAHs.

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