

The formation of benzene from acetylene clusters

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Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous in the interstellar medium (ISM)¹. The mechanism for their formation in the low temperature environment of the ISM is, as of yet, nonetheless a mystery. Understanding the mechanism of formation of complex molecules such as PAHs is a long-standing challenge, which has been drawing much attention for the past several decades.

Formation of the building blocks of PAHs upon ionization of van der Waals clusters will be presented. Results on small (up to 6 acetylene) van der Waals clusters, indicate that, due to the fact that the clusters possess a large amount of extra energy after ionization, a rich chemistry can occur². For example, after ionization, structures on the C₆H₆⁺ potential energy surface (PES) are accessible without barriers. Moreover, the formation of the basic building block of PAHs, namely the benzene cation, has been demonstrated by means of ab-initio molecular dynamic. The presence of spectator molecules has been proven to change the PES as well as to partake a catalytic role in the formation of the benzene cation.²

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References

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