Formation of PAH Clusters: Dynamics of Pure and N-substituted Cyclic Aromatic Hydrocarbon Formation in the Gas-Phase

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The processes by which complex organic molecules including large polycyclic aromatic hydrocarbons, known to be ubiquitous in the interstellar medium, and accounting for a significant portion of total carbon in the universe, is thus far unknown. Organic molecules are found in diverse astrophysical environments, most notably in molecular clouds and hot cores. Molecular ions, including positive and negative ions, are abundant in the high radiation fields present in star forming regions. Barrierless ion-molecule interactions may play a major role in guiding molecules towards each other and initiating reactions. We study neutral as well as ion-neutral condensation pathways to determine whether they are a viable means of forming large pure hydrocarbon molecules, nitrogen-containing carbonaceous chains, and cyclic compounds, by employing a variety of quantum chemical methods including coupled cluster and density functional theory methods. Where possible, the results from our calculations are compared with the results from experimental studies such as plasma discharge and ion-mobility experiments. We have investigated the process of growth, structural features, nature of bonding, reaction mechanisms, and spectroscopic properties of the ensuing products after pairing carbon, hydrogen, and nitrogen-containing precursors. Ab-initio molecular dynamics trajectory studies of the ion-neutral association pathways involving small PAHs spanning up to several nanoseconds at various temperatures reveal interesting details about the cluster formation process, and also their limitations.

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References

[1] *P. P. Bera*, Martin Head-Gordon, and Timothy J. Lee Astron & Astrophys. 535, A74 (2011)
[2] *P. P. Bera*, M. Head-Gordon, and T. J. Lee, 15, 2012-2023, Phys. Chem. Chem. Phys. (2013)
[3] P. P. Bera, R. Peverati, M. Head-Gordon, and T. J. Lee, Phys Chem Chem Phys, 17, 1859 (2015)
[4] Parker, Dangi, Yang, Kaiser, Bera and Lee, Astrophys J., 815, 115, (2015)
[5] R. Peverati, P. P. Bera, Martin Head-Gordon and Timothy J. Lee, Astrophys. J., 830, 128 (2016)
[6] T. Stein, P. P. Bera, T. J. Lee, and M. Head-Gordon, In preparation (2019)
[7] P. P. Bera, T. J. Lee, and A.G.G.M. Tielens, In preparation (2019)