Ultra-low-temperature reactions of C($^3P_0$) inside helium droplets

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Carbon atoms and ions are extremely abundant in the interstellar medium (ISM) [1]. The temperature of the ISM could be rather low. The lowest temperature found in space is 1 K [2]. In addition, it has been shown that there is no energy barrier for the reaction between atomic carbon and a broad variety of hydrocarbon molecules [3]. Therefore, the chemical inertness of molecules towards reaction with atomic carbon is an important property for them to reach a predominant abundance in the ISM.

Wehave initiated a project to study the reactivity of carbon atoms at ultra-lowtemperature. Atechnique to produce gas-phase carbon atoms with low kinetic energy suitable for the pick up by helium droplets has been developed [4]. It allows us to study the reactionsof carbon atoms with acetylene, benzene [5], naphthalene, anthracene, and coronene molecules in liquid helium droplets at T = 0.37 K. Mass spectrometry has been applied to characterize the products of the chemical reactions. Acalorimetric technique was used to evaluate the amount of energy released in the reaction. The geometries and vibrational frequencies of the stationary points of the reactants, intermediates, and possible product isomers were determined using the B3LYP hybrid functional and the 6-311+G(d,p) basis set. Our results suggest that PAH molecules with aromatic rings, which have at least 4 common carbon atoms, could be resistant towards the reaction with carbon atoms. This may result ina predominant abundance ofsuch PAH molecules in the ISM.

References

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