Formation mechanisms of triphenylene and 4- vinylacephenanthrylene in the interaction of 9-phenanthryl and vinilacetylene

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Polycyclic aromatic hydrocarbons (PAH) and soot, which generated in combustion processes, are harmful by-products. Therefore studying formation mechanisms of PAH from elementary chemical reactions initiating and propagating growth PAH at the molecular level, to successive nucleation of soot particles, particle coagulation and their surface growth, is very important research goal. The main task for understanding the molecular evolution of PAH is unraveling the elementary step of PAH expansion by one extra ring, which could be an additional six-member or five-member ring.

Formation mechanisms of indene and naphthalene from benzene were detailed studied in work [1]. Therefore, the question about expansion PAH from 1 to 2 rings can be considered solved. Some information about generation anthracene and phenanthrene in reaction naphthalene radicals with vinylacetylene is also available. Therefore, it seems interesting to investigate expansion PAH from 3 to 4 rings. Process of formation triphenylene and 4-vinylacephenanthrylene from 9-phenanthryl can be seen like a prototype of that elementary step evolution of PAH.

Main and some additional reaction channels of interaction 9-phenanthryl with vinylacetylene were defined in this work. Transition states and local minimums (wells) were optimized. G3 energy were calculated for them. Based on this data potential energy diagram was plotted (Fig. 1 shows some part of this diagram) and rate constants and relative yields of reaction were calculated.

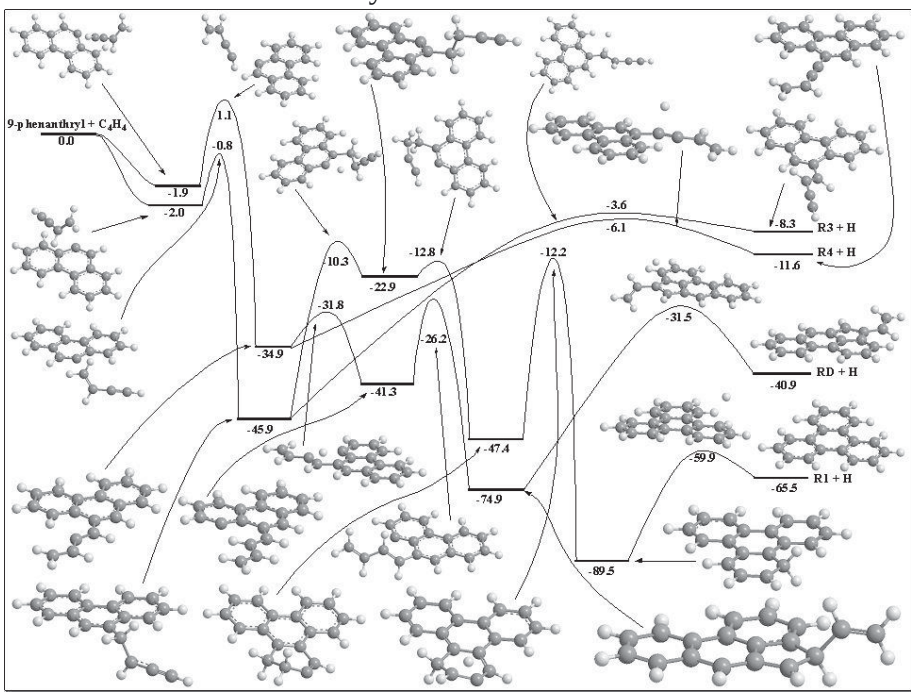

Fig.1 – The part of potential energy diagram with some main reaction channels

References:

1. Mebel, A.M.; Landera, A.; Kaiser, R.I.; Formation Mechanisms of Naphthalene and Indene From the Interstellar Medium to Combustion Flames. J. Phys. Chem. A. 2017, 121(5), 901-926