The reaction of 2-naphthyl with 1,3-butadiene: a theoretical study

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Recently obtained experimental and theoretical results of the investigation of the reaction of 1-naphthyl plus 1,3-butadiene defy the thesis that PAH growth is predominantly a high temperature phenomenon[1]. This work is devoted to theoretical investigation of 2-naphthyl + 1,3-butadiene reaction to complete the understanding of formation mechanisms of dihydrophenanthrene and dihydroanthracene in the reactions of n-naphthyl (n = 1, 2) with 1,3-butadiene. All intermediates and transition states, their vibrational frequencies and zero-point vibrational energies were calculated at G3(MP2,CC)//B3LYP/6-311G** theoretical level to generate the corresponding potential energy surface. Figure 1 represents the possible reaction pathways and scaled B3LYP potential energy surface. The results clearly indicate the possibility of the formation of both dihydrophenanthrene and dihydroanthracene in the title reaction.

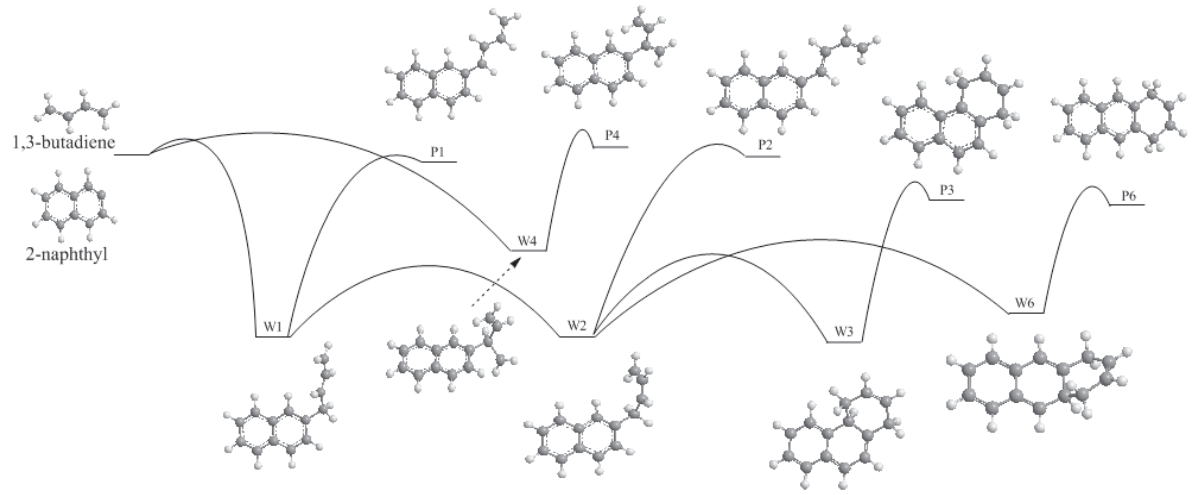

Figure 1. The pathway for the reaction of 2-naphthyl plus 1,3-butadiene depicting hydrogen-loss channels from various $C_{14}H_{13}$ adducts.

References:

1. Thomas, A. M., Lucas, M., Yang, T., Kaiser, R. I., Fuentes, L., Belisario-Lara, D., & Mebel, A. M. (2017). A Free Radical Pathway to Hydrogenated Phenanthrene in Molecular Clouds-Low Temperature Growth of Polycyclic Aromatic Hydrocarbons, *ChemPhysChem* 2017, 18, 1971-1976.