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Study of Carbon Isotopic Effects in Hydrocarbon Chains ZHE KAN, WANGYAO LI, MENGYAN SHEN, Univ of Mass - Lowell — ^{13}C has been a reliable candidate as an isotopic tracer in various research areas, such as chemical reactions, metabolic pathways, and molecule labeling. However, carbon isotope selectivity has been reported in recent hydrocarbon synthesis experiments by using the cobalt catalyzed Fischer-Tropsch method. Here, we present a theoretical study of the carbon isotopic effects in hydrocarbon chains. The theoretical methods include a Huckel-tight binding model, a configuration analysis, and quantum state perturbation theory. The electron vibrational energy in free ^{13}C atoms differs from that in free ^{12}C atoms and it is implemented in the Hamiltonian of each carbon atom ab-initially. Using the same amount of free ^{12}C and ^{13}C atoms provided as reactants, a possible configuration of mixed species bonded chains is analyzed in comparison with a configuration of the same species bonded chains. According to the calculations of these two configurations, noticeable differences in electron band structures and electron distributions are found. Moreover, the probability of converting free ^{12}C and ^{13}C atoms into a certain configuration of bonded chains is estimated through the methodology of quantum perturbation. The configuration involving only pure ^{12}C chains and ^{13}C chains is found to have the greatest possibility over any other configuration with mixed species bonded chains. It indicates that the same species tend to group together upon forming a hydrocarbon chain, this is in contradiction with a mechanism of random selection. This finding can provide a prediction and explanation of isotope selectivity in certain hydrocarbon synthesis experiments.

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