Abstract: Although the mechanisms of the pyrocarbon deposited by chemical vapor infiltration (CVI) using methane as carbon source have been researched widely through experiments, these mechanisms have not been studied deeply by quantum calculations which will help understand the CVI process from the molecular level. Based on the researches published previously, this work concluded the significant reactions during the conversion of methane to benzene involving species of C_1, C_2, C_4 and C_6, and all these reaction pathways were analyzed by theoretical and kinetic study. The geometry optimization and vibrational frequency analysis of all the chemical species and transition states (TS) were performed with B3LYP along with a basis set of 6-311+G(d,p), and Gaussian 09 software was used to study all the density functional theory (DFT). The rate constants were calculated by KiSThelP according to the conventional transition state theory (TST), and the Wigner method was applied to acquire the tunneling correction factors. Then the rate constants were fitted to the modified Arrhenius expression in the temperature range of 800-2000K. As for the barrierless reactions calculated in this paper, the rate constants were selected from the relating references. Through the energetic and kinetic calculations, the preferred pathways for benzene formation from methane can be determined. The results show that with the process proceeding, the reactions are becoming complicated multi-step ones gradually.