A theoretical study on the reaction of ethynyl radical with cyclopentadiene

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Abstract

The reaction of ground state ethynyl radical with cyclopentadiene at single-collision is investigated by combining reaction-paths predicting *ab initio* electronic structure calculations and RRKM theory to yield corresponding rate constants. The channels of isomerization and dissociation for each of the 15 collision complexes is characterized by employing the density functional B3LYP/cc-pVTZ and the CCSD(T)/CBS calculations, to optimize geometries and refine corresponding energies, respectively. With the facilitation of RRKM rate constants, through web of *ab initio* paths with 15 collision complexes, 200 more intermediates, and 47 H-, 100 H_2-, 3 C_2H_2-, 3 CCH_2-, dissociation products, we identify the most-probable paths down to around 14 species as the reaction mechanism. Subsequently, the rate equations of the reaction mechanisms are solved numerically so that the concentration evolutions for all species involved are obtained. This study predicts that C_2H + C_5H_6 reaction via any of the 15 collision complexes, would produce 3 major products, ethynyl-cyclopentadiene, 2-ethynyl-cyclopentadiene and 5-ethynyl-cyclopentadiene. Our investigation indicates that the barrierless and exoergic $C_2H(X^2\sum^+)$ + C_5H_6 (X^1A_1) reaction would be an efficient route for the potentially important ethynyl-cyclopentadiene in astrochemistry.