Reaction Mechanism of Nitromethane on the Graphene Surface: A Theoretical Study

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Abstract: To explore the effect of graphene on the reaction mechanism of nitromethane (NM), three kinds of initial reactions of NM on grapheme surface including the NM-methyl nitrite (MN) rearrangement reaction, the H-migration rearrangement reaction, and the C—N homolytic cleavage reaction were investigated by the ONIOM (our Own N-layer Integrated molecular Orbital and molecular Mechanics) method. Results show that the structures and energies of initial reaction transitions states of NM and reaction products are influenced by the graphene surface. The graphene surface makes the activation energy of three kinds of initial reactions decrease 13.4 kJ·mol^{-1}, increase 3.8 kJ·mol^{-1} and 5.4 kJ·mol^{-1} in the order. The orders of activation energies change from the C—N homolytic cleavage<the H-migration rearrangement<the NM-MN rearrangement to the NM-MN rearrangement<the C—N homolytic cleavage<the H-migration rearrangement. The reaction transition states and reaction products tend to form planar and eclipsed structures, respectively, leading to the maximization of interactions with graphene surface.

Key words: potential energy surface; activation energy; reaction transition states; our Own N-layer Integrated molecular Orbital and molecular Mechanics (ONIOM) method
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