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THEORETICAL STUDY OF THE FORMAMIDE DEGRADATION REACTION BY AU ATOM

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The related energy and multi-channel $CHONH_2$ degradation reaction potential energy surface under the catalysis of Au atom was studied, while its dynamic characterization have been investigated with density functional calculations. The geometries were fully optimized with the CCSD (T)//B3PW91 level. We can conclude two results: the calculated results shown that the main pathway of the CHONH2 degradation reaction under the catalysis of Au can give the main product P1 ($CO+NH_3$), while the minor product is P_2 (H_2+HNCO) and P_3 (H_2O+HNC). We calculated the rate constant of the main reaction pathway, the calculated dynamic characterization indicating that the rate constants have the positive temperature dependence; from the PESs, we can see the present invention, the singlet atom is the best catalysis and can catalyse the reaction better. The present invention studies may provide useful information on the issues of the reaction mechanism and product distributions.

Biography

Hongxia Liu has completed her PhD from Jilin University and Postdoctoral Studies from University of Massachusetts Amherst, School of Chemistry. She is serving as a Teacher at Inner Mongolia Normal University. She has published more than 30 papers in reputed journals. Her research studies include the theoretical and computational studies on the reaction mechanism, dynamics of the gas-phase reactions, molecule structure and surface catalysis. The results have been published on some scientific journals, such as J Comput Chem, ChemPhysLett, J Mol Struct (Theochem) et al.

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