Approximations of Statistical Quantum Mechanical model for atom-diatom insertion reaction studies

Ricardo Manuel García Vázquez[1], Maykel Márquez Mijares[1] and Lisandra Barrios Herrera[2]

[1]Department of Atomic and Molecular Physics, InSTEC-University of Havana, Cuba
[2]Department of Chemistry, University of Calgary, 2500 University Drive N. W., Calgary, Alberta, Canada T2N 1N4

Atom-diatom insertion reactions are characterized by the formation of an intermediate complex between reactants and product. Therefore, is possible to use statistical approaches in the theoretical investigation of this kind of reactions. The primary assumption of such techniques consists of the division of the whole process in two stages: the formation of the compound after the collision and its further fragmentation. The problem is resumed to the determination of a capture probabilities reactants and products. During the last decades, different approaches have been developed for estimate thus probabilities such as the Statistical Quantum Mechanical (SQM) model. Although this method introduces a considerable reduction of the computational time, in some cases (e.g., O+HCl, Si+OH) is quite complicated the use of the SQM approach, due to the existence of deep potential wells –which support many bound and quasi-bound states.

To address that challenges Barrios and coworkers introduced different approximations into the SQM model. In this work, we validate them by analyzing the typical insertion reaction $O+H_2$. Furthermore, we investigate, the Si+OH reaction, which plays a significant role in the formation of molecular SiO found in the interstellar medium. It is important to highlight that the standard SQM calculations for this system are extremely time-consuming, as a result, this study represents the first investigation of Si+OH system using the SQM approaches. From the results obtained we can conclude that the implemented approximations represent a tool of great benefit for the study of atom-diatom insertion reaction.