Effects of the Vibrational and Rotational Energy on Reaction Cross-Section in a Classical Trajectory Study of Atom-Diatomic Molecule Collisions

Hamzeh M. Abdel-Halim and Sawsan M. Jaafreh

The Hashemite University, Faculty of Science, Department of Chemistry, P.O. Box 330127, Zarqa 13133, Jordan

Reprint requests to Dr. H. M. A.-H.; E-mail: hamzehah@hu.edu.jo

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Effects of the initial vibrational and rotational energy of a diatomic molecule on reaction rates of atom-diatomic molecule reactions have been studied using classical trajectory calculations. The reaction probabilities, cross-sections and rate constants were calculated using the three-dimensional Monte-Carlo method. Equations of motion, which predict the positions and momenta of the colliding particles after each step in the trajectory, have been integrated numerically by the Runge-Kutta-Gill and Adams-Moulton methods. Morse potential energy surfaces were used to describe the interaction between the atom and each atom in the diatomic molecule. Several atom-diatomic molecule systems were studied. Variation of the reaction cross-section with both vibrational and rotational quantum numbers has been studied. For all systems studied, it was found that the cross-section increases with the vibrational quantum number. However, the effect of rotational quantum number on cross-section varies from one system to another.

Results obtained in the present work were compared with experimental data and/or with results obtained theoretically. Good agreements were observed with experimental and with theoretical results obtained by other investigators using different calculation methods.

Key words: Cross-Section; Vibration; Rotation; Atom-Diatom; Classical Trajectories.