Reaction Rate Constants from Classical Trajectories of Atom-Diatomic Molecule Collisions

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Classical trajectory calculations for various atom-diatomic molecules were preformed using the three-dimensional Monte Carlo method. The reaction probabilities, cross-sections and rate constants of several systems were calculated. Equations of motion, which predict the positions and momenta of the colliding particles after each step, 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 molecules. The results were compared with experimental ones and with other theoretical values. Good agreement was obtained between calculated rate constants and those obtained experimentally. Also, reasonable agreement was observed with theoretical rate constants obtained by other investigators using different calculation methods. The effects of the temperature, the nature of the colliding particles and the thermochemistry were studied. The results showed a strong dependence of the reaction rates on these factors.

Key words: Rates; Atom-Diatomic Molecule; Collisions; Classical Trajectories.