THE PREDICTION OF THERMOCHEMICAL AND KINETIC DATA FOR GAS PHASE REACTIONS. CURRENT STATUS

by

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In the past two decades there has been a remarkable growth in reliable experimental data on the Arrhenius parameters for elementary reactions. This includes reactions between neutrals (radicals, atoms, molecules) as well as unimolecular reactions involving these species. In the past decade a parallel and almost equally extensive body of data have begun to accumulate on ion-molecule reactions. The Transition State Theory of Chemical Reactions permits us to organize this experimental data into a relatively simple structure from which we can elucidate a number of simple generalizations which then permit us to make reasonably accurate estimates of the Arrhenius parameters for the rate constants of other, not yet measured elementary processes.

Our ability to use this predictive ability to develop multi-step mechanisms for complex chemical systems rests on a further experimental and empirical base of thermo-chemical data. Empirical additivity laws can be used to estimate entropies, heat capacities and heats of formation for radicals and large molecules with reasonable precision. Extension of these laws to charged species will be examined. We will in addition compare some elementary step reactions in plasmas with their analogues in chain reaction systems.