VARIFLEX MANUAL

(Version 1.0; July 16, 1999)

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Overview

VariFlex is a program package for estimating rate constants of several types of gas phase reactions. Its focus is the application of transition state theory with an accurate treatment of the flexibility of the interfragment modes for variable definitions of the reaction coordinate. Although aimed at calculating rates at this high level of sophistication for barrierless reactions, the package also allows convenient estimates of the rates using various alternative approaches such as phase space theory (PST), tight transition state theory, [i.e., with rigid rotor harmonic oscillator estimates (RRHO)], inverse Laplace transformations, and generic standard hydrocarbon estimates.

The following reaction types may be considered:

I. **Bimolecular association** reactions A + B => C.

II. **Unimolecular dissociation** reactions A => B + C.

III. **Bimolecular** reactions A + B => C + D.

IV. Competitive **multichannel** versions of each of the above, where more than one set of products is available, but involving only one complex or in the low pressure limit.

For each of these reaction types one may consider either **ionic** or **neutral** species.

The program focuses on the description of the temperature and/or pressure dependence of thermal reactions, where the reactants have a Boltzmann distribution of energies and angular momenta. However, microcanonical and *E/J* resolved dissociation rates are also generally available as a subset of the thermal calculations (that is, rates for reactants of specified energy, or specified energy and total angular momentum).

Methods are described for calculating

I. **High-pressure** limiting thermal rates evaluated at the ***T***, ***E***, and/or ***E/J*** resolved levels.

II. **Pressure-dependence** of thermal rates using the **RRKM** or **master equation** or Troe's **modified strong collision** formalism.

III. Zero-pressure and **low-pressure** limit thermal rates.

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