

Rice–Ramsperger–Kassel–Marcus (RRKM) theory

An improved form of Rice–Ramsperger–Kassel (RRK) theory in which account is taken of the way in which the various normal-mode vibrations and rotations contribute to reaction, and allowance is made for the zero-point energies. In this theory the energy ε^* in an energized molecule is classified as either active, $\varepsilon^{*\text{active}}$, or inactive, $\varepsilon^{*\text{inactive}}$. The rate depends upon $\frac{P(\varepsilon^{*\text{active}})}{N(\varepsilon^*)}$, where $N(\varepsilon^*)$ is the density of states having energy between ε^* and $\varepsilon^* + d\varepsilon^*$, and $P(\varepsilon^{*\text{active}})$ is the sum of the active quantum states of the activated complex. This extension of RRK theory brings it in line with transition-state theory.

Source:

PAC, 1996, 68, 149 (*A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996)*) on page 186