1 Key Results

General TST Expression for Rate Constant

$$k = \frac{k_B T}{h} \frac{(q_{ts\ddagger}/V)}{\prod(q_{react}/V)} \tag{1.1}$$

Factorised into Electronic and Nuclear Components

$$k = \frac{k_B T}{h} \left(\frac{[(q^{trans}_{ts\ddagger}/V) q^{rot}_{ts\ddagger} q^{vib}_{ts\ddagger}]}{\prod[(q^{trans}_{react}/V) q^{rot}_{react} q^{vib}_{react}]} \right) e^{-\frac{(E_{AB\ddagger} - \sum E_{react})}{k_B T}} \tag{1.2}$$

Translational Partition Function

$$q^{trans} = \frac{V}{\Lambda^3} \qquad \Lambda = \frac{h}{\sqrt{2\pi\, m\, k_B T}} \tag{1.3}$$

Rotational Partition Function

$$q^{rot} = \frac{\sqrt{\pi}}{\sigma} \left(\frac{T}{\Theta_A} \right)^{1/2} \left(\frac{T}{\Theta_B} \right)^{1/2} \left(\frac{T}{\Theta_C} \right)^{1/2} \tag{1.4}$$

$$\Theta_{A/B/C} = \frac{\hbar^2}{2 I_{A/B/C} k_B}$$

$$q^{rot,linear} = \frac{1}{\sigma} \frac{T}{\Theta} \tag{1.5}$$

$$\Theta = \frac{\hbar^2}{2 I k_B}$$

Vibrational Partition Function

$$q^{vib} = \prod_{i=1}^{n_{mode}} \frac{1}{1 - e^{-h\nu_i / k_B T}} \tag{1.6}$$

Constants and Conversion Factors | 2

Name	Symbol	Value
Boltzmann constant	k_B	1.380649×10^{-23} J K^{-1}
Planck constant	h	$6.62607015 \times 10^{-34}$ J s
hbar	$\hbar$	$h/2\pi = 1.05457182 \times 10^{-34}$ J s
Avogadro's number	N_A	$6.02214076 \times 10^{23}$ particles/mole
speed of light	c	29979245800 cm s^{-1}

Quantity	Reported Units	Required Units	Conversion process
Electronic energy, E	Hartree	J	$1\ E_h = 4.35974472 \times 10^{-18}$ J
Zero-point vib'l energy, ZPVE	kcal/mol	J	Multiply by 4.184 $\rightarrow$ kJ/mol Multiply by 1000 $\rightarrow$ J/mol Divide by $N_A = 6.02214076 \times 10^{23}$
Mass, m	g mol^{-1} (amu)	kg	Divide by 1000 $\rightarrow$ kg/mol Divide by $N_A = 6.02214076 \times 10^{23}$
Moment of inertia, I	amu Bohr^2	kg m^2	Convert amu to kg as above Convert Bohr to m, 1 Bohr = $0.529177249 \times 10^{-10}$ m
Vibrational frequency, ν	cm^{-1}	s^{-1}	Multiply by speed of light in cm s^{-1} c = 29979245800 cm s^{-1}