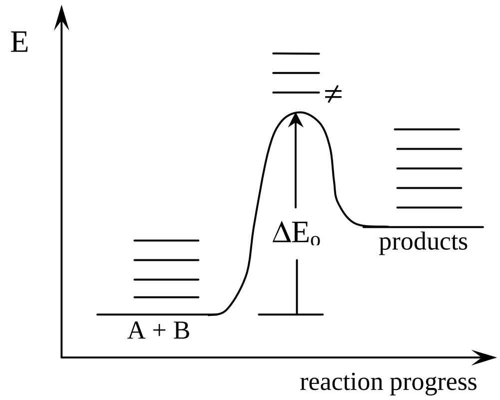
Thermodynamic Transition State Theory- Eyring Equation

$$A + B \rightarrow [AB]^{\neq} \rightarrow \text{products}$$

$$-\frac{d[A]}{dt} = k_2\,[A][B]$$



E = total electronic + rotation + vibration – reactive stretch

$$-\frac{d[A]}{dt} = \nu^{\neq}\,[AB]^{\neq}$$

$$k_2 = \nu^{\neq}\,\frac{[AB]^{\neq}}{[A][B]}$$

$$K_p = K_c \left(\frac{RT}{P^\circ}\right)^{\Delta n_g} \qquad \Delta n_g = -1$$

$$K_c = K_p \left(\frac{RT}{P^\circ}\right)$$

$$K_c = \frac{[AB]^{\neq}}{[A][B]} = \frac{q^{\neq\circ}/N_A}{(q_A^\circ/N_A)\,(q_B^\circ/N_A)} \left(\frac{RT}{P^\circ}\right) e^{-\Delta E_o/kT}$$

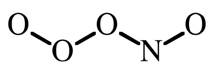
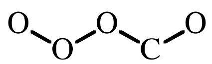
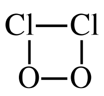
$$q^{\neq} = q_\nu^{\neq}\, q^{\neq\circ'}$$

$$q_\nu^{\neq} = \frac{1}{(1 - e^{-h\nu^{\neq}/kT})}$$

$$h\nu^{\neq}/kT << 1 \qquad e^{-h\nu^{\neq}/kT} = 1 - h\nu^{\neq}/kT + \ldots$$

$$q_\nu^{\neq} = \frac{kT}{h\nu^{\neq}} \qquad q^{\neq} = \frac{kT}{h\nu^{\neq}}\, q^{\neq\circ'}$$

$$k_2 = \frac{kT}{h}\,\frac{q^{\neq\circ'}/N_A}{(q_A^\circ/N_A)\,(q_B^\circ/N_A)} \left(\frac{RT}{P^\circ}\right) e^{-\Delta E_o/kT}$$

Reaction	E_a (kJ mol^{-1})	A exp (L mol^{-1} s^{-1})	A theory
$NO + O_3 \rightarrow NO_2 + O_2$ 	10.5	0.79×10^{12}	0.4×10^{12}
$NO_2 + CO \rightarrow NO + CO_2$ 	132	12.6×10^{12}	6.3×10^{12}
$2\,ClO \rightarrow Cl_2 + O_2$ 	0.0	0.063×10^{12}	0.01×10^{12}