

## Partition Functions and Units, Units, Units

$$q_t = \frac{(2\pi mkT)^{3/2}}{h^3} V \quad m \text{ in kg/molecule, } V \text{ in m}^3$$

$$V^\ominus = RT/P^\ominus \quad V^\ominus \text{ in m}^3$$

R = 8.31451 J/mol K	1 bar stand.state:	P <sup>⊖</sup> = 1.00x10 <sup>5</sup> N/m <sup>2</sup>
	1 atm stand.state:	P <sup>⊖</sup> = 1.01325x10 <sup>5</sup> N/m <sup>2</sup>
R = 0.0820578/1000 m <sup>3</sup> atm/mol K	1 bar stand.state:	P <sup>⊖</sup> = 0.98692 atm
	1 atm stand.state:	P <sup>⊖</sup> = 1.00 atm

$$q_t = \frac{V}{\Lambda^3} \quad \Lambda = \left( \frac{h^2}{2\pi mkT} \right)^{1/2} \quad \Lambda/\text{pm} = \frac{1749}{(T/\text{K})^{1/2} (\text{M/g mol}^{-1})^{1/2}}$$

$$\frac{q_{t,m}^\ominus}{N_A} = \frac{kT}{\Lambda^3 P^\ominus / \text{N/m}^2} = \frac{RT}{\Lambda^3 1000 \text{ L/m}^3 P^\ominus / \text{atm } N_A} = \Gamma (T/\text{K})^{5/2} (\text{M/g mol}^{-1})^{3/2}$$

$$\Gamma = \left( \frac{2\pi k}{N_A 1000 \text{ g kg}^{-1}} \right)^{3/2} \frac{k}{P^\ominus / \text{N/m}^2 h^3} = 0.025947 \quad \text{for 1 bar standard state}$$

$$= 0.025608 \quad \text{for 1 atm standard state}$$

$$50 \text{ g mol}^{-1} \text{ at } 298.2 \text{ K} \quad \frac{q_{t,m}^\ominus}{N_A} = 1.41 \times 10^7 \quad \cong 1 \times 10^7$$

$$\tilde{B} = 2 \text{ cm}^{-1} \quad \Theta_r = \frac{\tilde{B}hc}{k} = 2.878 \text{ K} \quad \frac{hc}{k} = 1.43877 \text{ cm K}$$

$$q_r = \frac{kT}{\sigma \tilde{B}hc} = \frac{207.2 \text{ cm}^{-1}}{\sigma \tilde{B}} = \frac{T}{\sigma \Theta_r} \cong 100$$

$$\text{at } 298.2 \text{ K} \quad q_v = \frac{1}{1 - e^{-h\nu_0/kT}} = \frac{1}{1 - e^{-\tilde{\nu}_0/207.2 \text{ cm}^{-1}}} = \frac{1}{1 - e^{-\Theta_v/T}} \quad \Theta_v = \frac{\tilde{\nu}_0 hc}{k}$$

$$\tilde{\nu}_0 = 150 \text{ cm}^{-1} \quad \Theta_v = 215.8 \quad q_v \cong 2$$

$$\tilde{\nu}_0 > 500 \text{ cm}^{-1} \quad \Theta_v > 719.4 \quad q_v = 1$$

$$1 \text{ cm}^{-1} = 11.962 \text{ J mol}^{-1} \quad 1 \text{ eV} = 1.602 \times 10^{-19} \text{ J} = 96.485 \text{ kJ mol}^{-1} = 8065.5 \text{ cm}^{-1}$$

T/K	100.0	298.2	500.0	1000.0	1500.0	2000.0
(kT/hc)/cm <sup>-1</sup>	69.5	207.226	347.5	695.0	1042.5	1390.1
kT/eV	0.009649	0.025695	0.04308	0.08617	0.1293	0.1723