Partition Functions and Units, Units, Units

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

$V_m^\circ = RT/P^\circ$ V_m° in m^3

$R = 8.31451\ J\ K^{-1}\ mol^{-1}$ 1 bar stand.state: $P^\circ = 1.00\text{x}10^5\ N\ m^{-2}$

1 atm stand.state: $P^\circ = 1.01325\text{x}10^5\ N\ m^{-2}$

$R = (0.0820578/1000)\ m^3\ atm\ K^{-1}\ mol^{-1}$ 1 bar stand.state: $P^\circ = 0.98692$ atm

1 atm stand.state: $P^\circ = 1.0000$ atm

$q_{t,m} = \dfrac{V_m}{\Lambda^3} = \dfrac{RT}{\Lambda^3 P}$ $\Lambda = \left(\dfrac{h^2}{2\pi mkT}\right)^{1/2}$ $\Lambda/\text{pm} = \dfrac{1749}{(T/K)^{1/2}(M/g\ mol^{-1})^{1/2}}$

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

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

$= 0.025608$ for 1 atm standard state

$50\ g\ mol^{-1}$ at 298.2 K $\dfrac{q_{t,m}^\circ}{N_A} = 1.41\text{x}10^7$ $\cong 1\text{x}10^7$

$\tilde{B} = 2\ cm^{-1}$ $\Theta_r = \dfrac{\tilde{B}hc}{k} = 2.878$ K $q_r = \dfrac{T}{\sigma\Theta_r}$ $\dfrac{hc}{k} = 1.43877$ cm K

$q_r = \dfrac{kT}{\sigma\tilde{B}hc} = \dfrac{207.2\ cm^{-1}}{\sigma\tilde{B}}$ at 298.2 K for $\tilde{B} = 2\ cm^{-1}$ $q_r \cong \dfrac{100}{\sigma}$

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at 298.2 K $q_V = \dfrac{1}{1 - e^{-h\nu_o/kT}} = \dfrac{1}{1 - e^{-\tilde{\nu}_o/207.2\ cm^{-1}}} = \dfrac{1}{1 - e^{-\Theta_v/T}}$ $\Theta_v = \dfrac{\tilde{\nu}_o hc}{k}$

$\tilde{\nu}_o = 150\ cm^{-1}$ $\Theta_v = 215.8$ K $q_V \cong 2$

$\tilde{\nu}_o > 500\ cm^{-1}$ $\Theta_v > 719.4$ K $q_V = 1$

$1 cm^{-1} = 11.962\ J\ mol^{-1}$ $1ev = 1.602\text{x}10^{-19}\ J = 96.485\ kJ\ mol^{-1} = 8065.5\ cm^{-1}$

T/K	100.0	298.2	500.0	1000.0	1500.0	2000.0
$(kT/hc)/cm^{-1}$	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