A Random Distribution of Formulas

$\mathcal{W} = \dfrac{\mathcal{N}!}{n_1!\, n_2!\, n_3! \ldots}$ $\qquad \ln x! = x \ln x - x \qquad e^{-x} \approx 1 - x \qquad Q = \dfrac{q^N}{N!}$

$q/N_A = (q_t/N_A)\, q_r\, q_v\, q_e \qquad n_i = \dfrac{\mathcal{N}}{Q} e^{-E_i/kT} \qquad U - U(0) = \dfrac{\sum n_i E_i}{\sum n_i} = -\dfrac{1}{Q}\left(\dfrac{\partial Q}{\partial \beta}\right)_V$

$$U - U(0) = \frac{-N}{q}\left(\frac{\partial q}{\partial \beta}\right)_V = -N\left(\frac{\partial \ln q}{\partial \beta}\right)_V = \frac{NkT^2}{q}\left(\frac{\partial q}{\partial T}\right)_V = \frac{nRT^2}{q}\left(\frac{\partial q}{\partial T}\right)_V = NkT^2\left(\frac{\partial \ln q}{\partial T}\right)_V$$

$S = \dfrac{k}{\mathcal{N}} \ln W_{max} = k \ln Q + \dfrac{U - U(0)}{T} \qquad S_m = \overline{S} = R \ln\left(\dfrac{q\, e}{N_A}\right) + RT\left(\dfrac{\partial \ln q}{\partial T}\right)_V$

$S = R \ln\left(\dfrac{(2\pi mkT)^{3/2}\, e^{5/2}\, V}{N_A\, h^3}\right) \qquad A - A(0) = -kT \ln Q \qquad P = kT\left(\dfrac{\partial \ln Q}{\partial V}\right)_T$

$G - G(0) = -kT \ln Q + kTV\left(\dfrac{\partial \ln Q}{\partial V}\right)_T \qquad G - G(0) = -nRT \ln\left(\dfrac{q}{N}\right) \qquad q_t = \dfrac{(2\pi mkT)^{3/2}}{h^3} V$

$\dfrac{q^\circ_{t,m}}{N_A} = \Gamma\, (T/K)^{5/2}\, (M/g\ mol^{-1})^{3/2} \qquad \Gamma = \left(\dfrac{2\pi k}{N_A 1000 g\ kg^{-1}}\right)^{3/2} \dfrac{k}{P^\circ/_{N/m^2}\, h^3} = 0.025947$ at 1 bar

$q_r = \dfrac{kT}{\sigma \tilde{B}hc} = \dfrac{T}{\sigma \Theta_{rot}}$ or $q_r = \dfrac{\pi^{1/2}}{\sigma}\left(\dfrac{kT}{\tilde{A}hc}\right)^{1/2}\left(\dfrac{kT}{\tilde{B}hc}\right)^{1/2}\left(\dfrac{kT}{\tilde{C}hc}\right)^{1/2} = \dfrac{\pi^{1/2}}{\sigma}\left(\dfrac{T^3}{\Theta_{rot,A}\, \Theta_{rot,B}\, \Theta_{rot,C}}\right)^{1/2} \qquad \Theta_{rot} = \dfrac{\tilde{B}hc}{k}$

$G - G(0) = -RT \ln\left(\dfrac{kT}{\sigma \tilde{B}hc}\right) = -RT \ln\left(\dfrac{T}{\sigma \Theta_{rot}}\right)$ or $G - G(0) = -RT \ln\left(\dfrac{\pi^{1/2}}{\sigma}\left(\dfrac{T^3}{\Theta_{rot,A}\, \Theta_{rot,B}\, \Theta_{rot,C}}\right)^{1/2}\right)$

$q_v = \dfrac{e^{-h\nu_o/2kT}}{1 - e^{-h\nu_o/kT}}$ or $q_v = \dfrac{1}{(1 - e^{-h\nu_o/kT})} = \dfrac{1}{(1 - e^{-hc\tilde{\nu}_o/kT})} = \dfrac{1}{1 - e^{-\Theta_{vib}/T}} \rightarrow \dfrac{kT}{h\nu_o} \qquad \Theta_{vib} = \dfrac{hc\,\tilde{\nu}_o}{k}$

$U - U(0) = \dfrac{Nh\nu_o\, e^{-h\nu_o/kT}}{1 - e^{-h\nu_o/kT}} = \dfrac{Nk\, \Theta_{vib}\, e^{-\Theta_{vib}/T}}{1 - e^{-\Theta_{vib}/T}} \qquad G - G(0) = RT \ln(1 - e^{-h\nu_o/kT}) = RT \ln(1 - e^{-\Theta_{vib}/T})$

$S_{rot} = R \ln\left(\dfrac{kT}{\sigma \tilde{B}hc}\right) + R$ or $S_{rot} = R \ln \dfrac{\pi^{1/2}}{\sigma}\left(\dfrac{kT}{\tilde{A}hc}\right)^{1/2}\left(\dfrac{kT}{\tilde{B}hc}\right)^{1/2}\left(\dfrac{kT}{\tilde{C}hc}\right)^{1/2} + \dfrac{3}{2} R$

$S_{vib} = -R \ln(1 - e^{-h\nu_o/kT}) + \dfrac{Nh\nu_o}{T}\dfrac{e^{-h\nu_o/kT}}{(1 - e^{-h\nu_o/kT})} \qquad q = \dfrac{(2\pi mkT)^{3/2}}{h^3} V \dfrac{kT}{\sigma \tilde{B}hc} \dfrac{1}{(1 - e^{-hc\tilde{\nu}_o/kT})}\, g_e\, e^{-D_o/kT}$

$$K_p = \frac{\left(q^\circ_C/N_A\right)^c \left(q^\circ_D/N_A\right)^d}{\left(q^\circ_A/N_A\right)^a \left(q^\circ_B/N_A\right)^b} e^{-\Delta E_o/RT}$$

$$K_p = \left(\frac{m_{AB}\, m_C}{m_A\, m_{BC}}\right)^{3/2} \left(\frac{\dfrac{1}{\sigma_{AB}\tilde{B}_{AB}}}{\dfrac{1}{\sigma_{BC}\tilde{B}_{BC}}}\right) \left(\frac{\dfrac{1}{1 - e^{-hc\tilde{\nu}_o(AB)/kT}}}{\dfrac{1}{1 - e^{-hc\tilde{\nu}_o(BC)/kT}}}\right) \left(\frac{g_{AB}\, g_C}{g_A\, g_{BC}}\right) e^{-\Delta E_o/RT}$$

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

$$k_2 = \frac{kT}{h}\left(\frac{RT}{P^\circ}\right) e^{-\Delta G^{\circ\neq}/RT} = \frac{kT}{h}\left(\frac{RT}{P^\circ}\right) e^{\Delta S^{\circ\neq}/R}\, e^{-\Delta H^{\circ\neq}/RT} \qquad E_a = \Delta H^{o\neq} + 2RT$$

$$k_2 = \frac{kT}{h}\left(\frac{RT}{P^\circ}\right) e^2\, e^{\Delta S^{\circ\neq}/R}\, e^{-E_a/RT}$$

$$2d_{hkl} \sin\theta = n\lambda \qquad d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}} \qquad \sin\theta = \frac{\lambda}{2a}\sqrt{h^2+k^2+l^2} \qquad M = h^2+k^2+l^2$$

$$\Delta\phi = 2\pi\,(hx + ky + lz) \qquad F_{hkl} = F_{hkl} = f_B + f_A\, e^{2\pi i\,(hx + ky + lz)} \qquad F_{hkl} = \sum_{i=1}^{N} f_i\, e^{2\pi i\,(hx_i + ky_i + lz_i)}$$

BCC (I): $(h + k + l)$ even FCC (F): all even or all odd $d_{hkl} = \frac{1}{d^*_{hkl}} = \frac{M\lambda}{DF}$

$c = 2.998\text{x}10^{8}$ m s^{-1} $e = 1.602\text{x}10^{-19}$C $k = 1.381\text{x}10^{-23}$ J K^{-1}

R = 8.314 J K^{-1}mol^{-1}=0.08314 bar L K^{-1}mol^{-1} = 0.08206 L atm K^{-1} mol^{-1}

$h = 6.626\text{x}10^{-34}$ J s $\hbar = 1.054\text{x}10^{-34}$ J s

$N_A = 6.022\text{x}10^{23}$ mol^{-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}

1H = 2625.5 kJ mol^{-1} = 27.211 eV a_o = 0.529Å = 52.9 pm

T/K	100.0	298.2	500.0	1000.0	1500.0	2000.0
kT/hc/cm^{-1}	69.50	207.226	347.5	695.0	1042.5	1390.1
kT/eV	0.009649	0.025695	0.04308	0.08617	0.1293	0.1723
(kT/h)/s^{-1}	$2.084\text{x}10^{12}$	$6.212\text{x}10^{12}$	$1.042\text{x}10^{13}$	$2.084\text{x}10^{13}$	$3.13\text{x}10^{13}$	$4.17\text{x}10^{13}$