2.1 a) $T = 300\,K$

$k_B T = 4.14 \times 10^{-21}\,J$

b) $k_B T = 4.14 \times 10^{-21}\,J \,/\, 1.602 \times 10^{-19}\,J/eV$

$= 0.026\,eV$

c) Boltzmann factor

$e^{-E/k_B T} \approx e^{-173} = 6.8 \times 10^{-76} \approx 0$

H_2 <u>not</u> dissociated at room temperature

d) $T = \frac{E}{k_B} = \frac{4.5\,eV}{k_B} = 52170\,K$

e) $e^{-E/k_B T} = e^{-3.8 \times 10^{-3}} \approx 1$

rotational energy levels are excited

2.2 a) $Z = e^{\beta\varepsilon} + e^{2\beta\varepsilon}$

$$P_1 = \frac{e^{\beta\varepsilon}}{e^{\beta\varepsilon} + e^{2\beta\varepsilon}} = \frac{1}{1 + e^{\beta\varepsilon}}$$

b) $$P_2 = \frac{e^{2\beta\varepsilon}}{e^{\beta\varepsilon} + e^{2\beta\varepsilon}} = \frac{e^{\beta\varepsilon}}{1 + e^{\beta\varepsilon}}$$

c) $$\langle E \rangle = -P_1 \varepsilon - P_2 2\varepsilon$$

$$= \frac{-\varepsilon - 2\varepsilon e^{\beta\varepsilon}}{1 + e^{\beta\varepsilon}} = -2\varepsilon + \frac{\varepsilon}{1 + e^{\beta\varepsilon}}$$

d) $T \to 0$, $\beta\varepsilon \to \infty$: $\langle E \rangle = -2\varepsilon$ ground state

$T \to \infty$, $\beta\varepsilon \to 0$: $\langle E \rangle = -2\varepsilon + \varepsilon/2 = -3/2\,\varepsilon$

e) $$C = \frac{d}{dT}\langle E \rangle = \frac{-\varepsilon}{(1 + e^{\beta\varepsilon})^2} e^{\beta\varepsilon} \left(\frac{-\varepsilon}{k_B T^2} \right)$$

$$= k_B \frac{e^{\beta\varepsilon}}{(1 + e^{\beta\varepsilon})^2} \left(\frac{\varepsilon}{k_B T} \right)^2$$

f) $T \to 0$, $\beta\varepsilon \to \infty$: $C = 0$

$T \to \infty$, $\beta\varepsilon \to 0$: $C = 0$

g) $C = k_B \frac{e^x}{(1+e^x)^2} x^2 \qquad x = \beta\varepsilon$

maximum w.r.t. x

$$\frac{d}{dx}\left(\frac{C}{k_B}\right) = \frac{x^2 e^x}{(1+e^x)^2} + \frac{2x e^x}{(1+e^x)^2} - \frac{2x^2 e^x}{(1+e^x)^3} e^x = 0$$

$$0 = x + 2 - 2x\frac{e^x}{1+e^x} = 2 + x\frac{1+e^x-2e^x}{1+e^x}$$

$$\frac{2}{x} = \frac{e^x-1}{e^x+1} \Rightarrow x_m = 2.399$$

$$\frac{\varepsilon}{k_B T_m} = 2.399 \qquad k_B T_m = 0.416\,\varepsilon$$

h) $C_{max} = k_B \times 0.439$