Problem 1

Average energy of an oscillator is

$$\langle E \rangle = \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1} \quad ; \quad k_B = \frac{1}{11,600}\frac{eV}{K}$$

At $T = 100K$:

$$\frac{\hbar\omega}{k_BT} = \frac{0.01 eV}{100K \cdot eV} 11,600 K = 1.16$$

$$\langle E \rangle = \frac{\hbar\omega}{e^{1.16}-1} = 0.457\,\hbar\omega = 0.457\frac{\hbar\omega}{k_BT}\cdot k_BT = 0.53\,k_BT$$

$$\boxed{\langle E \rangle = 0.53\,k_BT} \quad (a)$$

(b) The Einstein temperature for this oscillator is:

$$T_E = \frac{\hbar\omega}{k_B} = \frac{0.01 eV}{eV} \times 11,600K = 116\,°K$$

$$\langle E \rangle = \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1} = \frac{k_BT_E}{e^{T_E/T}-1} = \frac{T_E}{T}\frac{1}{e^{T_E/T}-1}(k_BT)$$

So we need: $f(T) = \frac{T_E}{T}\frac{1}{e^{T_E/T}-1} > 0.9$; note that as $T \to \infty$, $f(T) \to 1$

let $x = T/T_E \Rightarrow f(x) = \frac{1}{x}\frac{1}{e^{1/x}-1} > 0.9$. Use calculator

x	f(x)
3	0.84
5	0.903
10	0.95

$\Rightarrow x \gtrsim T/T_E > 5 \Rightarrow \boxed{T > 5T_E = 580\,°K}$

(c) Need $f(x) < 0.01$. For small x, $f(x) \cong \frac{1}{x}e^{-1/x} < 0.01$

x	f(x)
0.25	0.07
0.1	0.0005

$x = \frac{T}{T_E} < 0.1 \Rightarrow \boxed{T < 0.1T_E = 11.6\,°K}$

Problem 2

$$E_{im} = I(X) - 3.62\,eV$$

is energy we pay to do $XCl \longrightarrow X^+ \; Cl^-$

we gain Coulomb energy $U(r) = -\frac{ke^2}{r}$

$\Rightarrow$ need $U(r) + E_{im} < 0 \Rightarrow I(X) < 3.62\,eV + \frac{ke^2}{r}$

For $r = 2.5\,\mathring{A}$, $ke^2 = 14.4\,eV\mathring{A} \Rightarrow$

$$\boxed{I(X) < 3.62\,eV + 5.76\,eV = 9.38\,eV}$$

(b) If the dissociation energy is $2\,eV \Rightarrow$

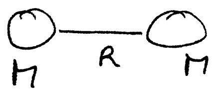
$$\boxed{I(X) = 9.38\,eV - 2\,eV = 7.38\,eV}$$

assuming no repulsion.

(c) If the ionization energy is only $5\,eV \Rightarrow$

$$\boxed{E_{repulsion} = 7.38\,eV - 5\,eV = 2.38\,eV}$$

Problem 3



(a) According to classical equipartition thm, $C_V = \frac{1}{2} k_B$ per degree of freedom

Translation: $\frac{3}{2} k_B$, Rotation: k_B, Vibration: k_B

A degree of freedom doesn't contribute if $k_B T <<$ characteristic energy, gives classical value if $k_B T >>$ characteristic energy

$$\Rightarrow \quad k_B T_1 << \hbar\omega << k_B T_2$$

(b) Moment of inertia: $I = \frac{1}{2} M R^2$. $E_{0r} \equiv \frac{\hbar^2}{2I} = \frac{\hbar^2}{MR^2}$

Rotational energy: $E_r(l) = \frac{\hbar^2}{2I} l(l+1) \equiv E_{0r} \cdot l(l+1)$

Vibrational energy $E_v(v) = \hbar\omega(v + \frac{1}{2})$

Selection rules: $v = 0 \to v = 1$ for vibrational states, starting at $v = 0$

$l \to l+1$ or $l \to l-1$ for rotational state

$$E(v=0, l=3) = \frac{\hbar\omega}{2} + E_{0r} \cdot 3 \cdot 4 = \frac{\hbar\omega}{2} + 12 E_{0r}$$

$$E(v=1, l=4) = \frac{\hbar\omega}{2} + \hbar\omega + E_{0r} \cdot 4 \cdot 5 = \frac{3}{2}\hbar\omega + 20 E_{0r}$$

$$E(v=1, l=2) = \frac{3}{2}\hbar\omega + E_{0r} \cdot 2 \cdot 3 = \frac{3}{2}\hbar\omega + 6 E_{0r}$$

So photons absorbed have energy:

$$E_1 = E(v=1, l=4) - E(v=0, l=3) = \boxed{\hbar\omega + 8 E_{0r}}$$

$$E_2 = E(v=1, l=2) - E(v=0, l=3) = \boxed{\hbar\omega - 6 E_{0r}}$$

(c) For $M = 938$ MeV, $R = 1 Å$, $E_{0r} = \frac{\hbar^2}{2I} = \frac{\hbar^2}{MR^2} = 0.0042$ eV

For $\hbar\omega = 0.05$ eV

$$E_1 = 0.05 \text{ eV} + 8 \times 0.0042 \text{ eV} = \boxed{0.084 \text{ eV}}$$

$$E_2 = 0.05 \text{ eV} - 6 \times 0.0042 \text{ eV} = \boxed{0.025 \text{ eV}}$$