1.	The theoretical lattice energy equation is shown.

$$U = \frac{NM_{NaCl}Z^2e^2}{4\pi\varepsilon_o r_o}\left(1-\frac{1}{n}\right)$$

a.	Which factors are dependent on the identities of the atoms that make up the solid?

Z = charge on ions
r_0 = distance between cation and anion
n = compressibility for the solid
M = Madelung constant (technically depends on packing geometry, which is somewhat determined by size/shape of atoms

b.	What is a Madelung constant? Why can the same Madelung constant be used for seemingly different substances?

A Madelung constant is relates all the charged particles in a lattice with each other- It describes the geometries of all columbic interactions within a lattice. The Madelung constant is determined solely by the geometry of ions in the structure so materials with the same geometries, the same geometric relationship between ions in the lattice can use similar Madelung constants, regardless of the charge on the ions.

2.	Use Figure 4-2 in Cotton as a guide and write out balanced chemical equations for each step in the Born-Haber cycle of MgO. Using the given data, determine the lattice energy.

For Mg (s), Δ Hsub = +148 kJ/mol
Bond dissociation energy for O_2 = +499 kJ/mol
1st ionization energy for Mg = +738 kJ/mol;
2nd ionization energy for Mg = +1450 kJ/mol;
1st electron affinity enthalpy for O = –141 kJ/mol;
2nd electron affinity enthalpy for O = +748 kJ/mol
For MgO (s), enthalpy of formation = –602 kJ/mol

**$Mg_{(s)}$ + ½ $O_{2(g)}$ → $Mg_{(g)}$ + ½ $O_{2(g)}$	[ΔH_{vap}]**
**$Mg_{(g)}$ + ½ $O_{2(g)}$ → $Mg_{(g)}$ + $O_{(g)}$	[ΔH_{diss}]**
**$Mg_{(g)}$ + $O_{(g)}$ → $Mg^{2+}_{(g)}$ + $O_{(g)}$	[ΔH_{ion}]**
**$Mg^{2+}_{(g)}$ + $O_{(g)}$ → $Mg^{2+}_{(g)}$ + $O^{2-}_{(g)}$	[ΔH_{EA}]**
**$Mg^{2+}_{(g)}$ + $O^{2-}_{(g)}$ → $MgO_{(s)}$	[U]**
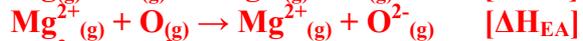
Lattice Enthalpy = 3845 kJ/mol

3.	Study the unit cell drawings found in Cotton chapter 4 for NaCl, zinc blende, rutile, CsCl and fluorite. Now by the location of each atom type in the unit cell (corner, edge, face or internal) add up all the contributions from these atoms to show how the empirical formula is arrived at.

Hint: corner atoms are shared by eight unit cells, edges are shared by four unit cells, face atoms are shared by two unit cells and internal atoms belong to only one unit cell.

NaCl
Cl: 4 face + 8 corner = (4 x 0.5) + (8 x 0.125) = 4
Na: 1 center + 12 edge = (1 x 1) + (12 x 0.25) = 4

Zinc Blende (ZnS)
S: 6 face + 8 corner = (6 x 0.5) + (8 x 0.125) = 4
Zn: 4 interior = 4

Rutile (TiO$_2$)
Ti: 8 corner + 1 interior = (8 x 0.125) + (1 x 1) = 2
O: 4 face + 2 interior = (4 x 0.5) + (2 x 1) = 4

CsCl
Cl: 1 center = 1
Cs: 8 corner = (8 x 0.125) =

Fluorite (CaF$_2$)
Ca: 8 corner + 6 face = (8 x 0.125) + (6 x 0.5) = 4
F: 8 interal = 8

4.	Derive the radius ratio ideal value for NaCl type structures (CN=6)
	Hint: see the figure to the right.
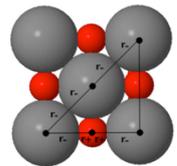
The plane is just the face of the unit cell.

$$4r^- = \left(2r^- + 2r^+\right)\sqrt{2}$$

$$\frac{r^+}{r^-} = \frac{2}{\sqrt{2}} - 1 = 0.414$$

5.   Using the radius ratio approach, predict coordination numbers for LiF, LiCl, LiBr, NaBr and KBr. Explain using words and figures (*Hint: consider geometry, size of ions and stability*) why these differences in coordination numbers exist.

* can do these anion:cation or cation:anion. Just make sure to use the right chart…

LiF: 0.60/1.35 = 0.444 → NaCl type CN=6
LiCl: 0.60/1.67 = 0.359 → ZnS type CN=4
LiBr: 0.60/1.95 = 0.307 →ZnS typte CN=4
NaBr: 0.96/1.95 = 0.493 → NaCl type CN=6
KBr: 1.33/1.95 = 0.682 → NaCl type CN=6

Assume ions are spherical and ion size determines packing, cations will surround themselves with as many anions as possible and vice versa. For a specific structure, there is a minimum allowable value for the structure to be stable – must optimize the cation and anion interactions otherwise the structure will not be stable. The differences in coordination number arise from the number of anions that can fit around a given cation in a certain geometry based on the size of the anion and cation.

6.   Using drawings, show the difference between cubic and hexagonal close packing.
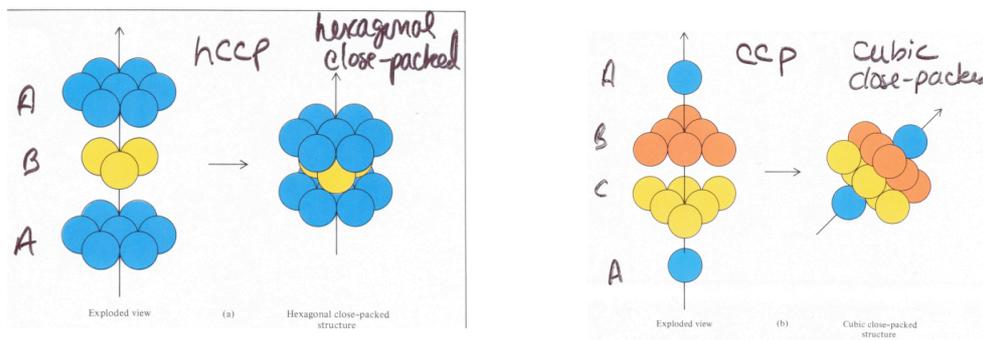
7.   What are the three types of cubic unit cells? Sketch them, and describe the similarities/differences

All are cubic, all have atoms in the corners
Body centered has an atom in the middle, face centered has an atom on each face but not in the middle. Simple cubic does not have anything else between the vertices.