AT Chemistry
2015

POGIL on CHEMICAL BONDING

Part II: Born Haber Cycle and Bond Energies

The formation of a binary ionic compound can be viewed as occurring in several steps with each step having its own heat of reaction. The sum of the steps yields the net reaction and the sum of the ΔH's for each step adds up to the ΔH for the reaction (remember Hess' law?). The sequence of reactions is known as the Born Haber cycle.

key idea: ***lattice energy*** - the energy released when an ionic solid is formed from its gaseous ions. This is the most favorable energy term in the process.

Let's consider the steps involved in the formation of solid potassium chloride from its elements at standard conditions.

First, what are standard conditions?

$25^{o}C$ (298K) and 1 atm (101.3 kPa)

Write the net equation for the formation of potassium chloride from its elements under standard conditions (this means include the phases of reactants and products under standard conditions):

$K(s) + 1/2Cl_2(g) \rightarrow KCl(s)$

Keep in mind that in the final step of our process, we want to react gaseous ions to form our solid salt (involving the lattice energy!).

1. The first step is to take our metal in its standard state and sublime it.

   Is this a physical or chemical change? physical

   Is this change endothermic or exothermic? endothermic

   Is this change energetically favorable? no

   Write an equation representing this reaction and include the energy term as H_{sub}:

$K(s) + H_{sub} \rightarrow K(g)$

2. The next step is to take our metal vapor and ionize it.

   Are electrons removed from potassium or added to potassium to result in a "stable" ion?

   removed

   How many electrons? one

   What is the energy needed to remove this electron called? ionization energy

   Does this involve and endothermic or exothermic reaction? endothermic

   Is this change energetically favorable? no

   Write an equation representing this reaction and include the energy term as IE_1

   $K(g) + IE_1 \rightarrow K^+(g)$

   We now have our gaseous metal ion.

3. Now we consider our nonmetal reactant.

   Is our nonmetal in the gas phase at standard conditions? yes

   What must we do to get one atom of our nonmetal in the gas phase? Or one mole of atoms of our nonmetal in the gas phase?

   Break the bond between the chlorine atoms in the chlorine molecule

   That's right (I knew you would figure it out)! We need to break the bond between the two chlorine atoms. The energy needed to do this is called bond energy (how did they get that name?!?) and is given in kJ/mol. Now to get one mole of chlorine gas atoms, how many moles of chlorine gas do we need to break apart? one-half

   Is bonding breaking endothermic or exothermic? endothermic

   Is this energetically favorable? no

   Now write an equation that shows this change and include the energy term as H_{bond}:

   $1/2Cl_2(g) + H_{bond} \rightarrow Cl(g)$

4. We now have a single nonmetal atom in its gaseous phase. Next we need to ionize it.

   Does chlorine gain or lose electrons to form a "stable ion"? gain

   How many electrons? one

   What is the process called that adds an electron to a gaseous atom? electron affinity

   Is this process endothermic or exothermic? exothermic

   Is this process energetically favorable? yes

   Now write an equation that shows this change and include the energy term as EA_1:

   $$Cl(g) + e^- \rightarrow Cl^-(g) + EA_1$$

   We now have our gaseous nonmetal ion.

5. The last step in this process involves combining our gaseous ions to produce our solid ionic compound (potassium chloride). As mentioned previously, this is the most energetic step and will drive the overall reaction.

   Is this step endothermic or exothermic? **very exothermic**

   Is this step energetically favorable or unfavorable? favorable

   Write an equation for this reaction and include the energy term as LE:

   $$K^+(g) + Cl^-(g) \rightarrow KCl(s) + LE$$

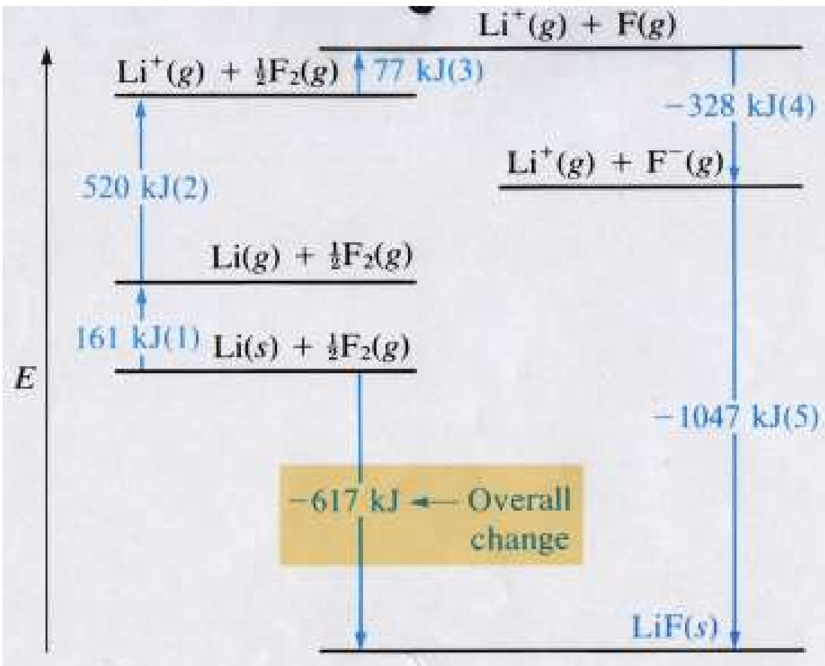
6. Now let's add the five individual reactions and their ΔH's to get the net reaction and the net ΔH:

reaction		ΔH (kJ/mol)
1. $K(s) \rightarrow K(g)$	*Esublimation =*	*+64 kJ*
2. $K(g) \rightarrow K^+(g) + e^-$	*IE =*	*+419 kJ*
3. $1/2Cl_2(g) \rightarrow Cl(g)$	Bond Energy =	+120 kJ/mol (X1/2)
4. $Cl(g) + e^- \rightarrow Cl^-(g)$	EA =	-349 kJ
5. $K^+(g) + Cl^-(g) \rightarrow KCl(s)$	lattice energy =	-690 kJ

NET: $K^+(g) + Cl^-(g) \rightarrow KCl(s)$ ΔH =

Note: the higher the charge on each ion, the greater the lattice energy. This counteracts the higher endothermic IE's resulting in a more stable ionic crystal

Below is a Born-Haber energy diagram for the formation of lithium fluoride from its elements:



7. Write the reactions for each step, the ΔH for each step, and then add to give the net reaction and net ΔH as on the previous page.

$Li(s) + H_{sub} \rightarrow Li(g)$	161 kJ
$Li(g) + IE_1 \rightarrow Li^+(g)$	520 kJ
$1/2F_2(g) + H_{bond} \rightarrow F(g)$	154/2 = 77 kJ
$F(g) + e^- \rightarrow F^-(g) + EA_1$	-328 kJ
$Li^+(g) + F^-(g) \rightarrow LiF(s) + LE$	-1047 kJ
$Li(s) + 1/2F_2(g) \rightarrow LiF(s)$	-617 kJ

Text problem 56: Use the following data to estimate the ΔH_f^o for magnesium fluoride

$$Mg(s) + F_2(g) \rightarrow MgF_2(s)$$

Lattice energy	-2913 kJ/mol
First ionization energy of Mg	735 kJ/mol
Second ionization energy of Mg	1445 kJ/mol
Electron affinity of F	-328 kJ/mol
Bond Energy of F_2	154 kJ/mol
Enthalpy of sublimation for Mg	150.kJ/mol

$Mg(s) \rightarrow Mg(g)$	150 kJ	H sublimation
$Mg(g) \rightarrow Mg^+(g) + e^-$	735 kJ	IE1
$Mg^+(g) \rightarrow Mg^{2+}(g) + e^-$	1445 kJ	IE2
$2(g) \rightarrow 2F(g)$	154 kJ	bond energy
$F(g) + e- \rightarrow F^-(g)$	-328 kJ	EA
$F(g) + e- \rightarrow F^-(g)$	-328 kJ	EA
$Mg^{2+}(g) + 2F^-(g) \rightarrow MgF2(s)$	-2913 kJ	LE
$Mg(s) + F_2(g) \rightarrow MgF_2(s)$	-1085 kJ	ΔH

Text problem 59: LiI(s) has a heat of formation of -272 kJ/mol and a lattice energy of -735 kJ/mol. The ionization energy of Li(g) is 520. kJ/mol, the bond energy of $I_2(g)$ is 151 kJ/mol, and the electron affinity of I(g) is -295 kJ/mol. Use these data to determine the heat of sublimation of Li(s).

$Li(s) \rightarrow Li(g)$	?
$Li(g) \rightarrow Li^+(g) + e^-$	520 kJ
$1/2I_2(g) \rightarrow I(g)$	151 kJ/2 = 75.5 kJ
$I(g) + e^- \rightarrow I^-(g)$	-295 kJ
$Li^+(g) + I^-(g) \rightarrow LiI(s)$	-735 kJ
$Li(s) + 1/2I_2(g) \rightarrow LiI(s)$	-272 kJ

? = 163 kJ

Bond Energies and ΔH

Bond energy = average value (assume bond is not sensitive to environment)

$$\Delta H = \underset{\text{(endothermic)}}{\sum D(\text{bonds broken})} - \underset{\text{(exothermic)}}{\sum D(\text{bonds formed})}$$

8. Using bond energy data calculate ΔH for the following reaction. Compare this to the ΔH calculated using thermodynamic values.

$$CH_4 + 4F_2 \rightarrow CF_4 + 4HF$$

ΔH = [(4)(C-H) + (4)(F-F)] - [(4)(C-F) + (4)(H-F)]

= [(4)(413) + (4) 154)] - [(4)(485) + (4)(565)]

= -1932 kJ