Enthalpy of Reaction from Bond Energies

Table 8.4 Average Bond Energies (kJ/mol)

Single Bonds						*Multiple Bonds*	
H—H	432	N—H	391	I—I	149	C=C	614
H—F	565	N—N	160	I—Cl	208	C≡C	839
H—Cl	427	N—F	272	I—Br	175	O=O	495
H—Br	363	N—Cl	200			C=O*	745
H—I	295	N—Br	243	S—H	347	C≡O	1072
		N—O	201	S—F	327	N=O	607
C—H	413	O—H	467	S—Cl	253	N=N	418
C—C	347	O—O	146	S—Br	218	N≡N	941
C—N	305	O—F	190	S—S	266	C≡N	891
C—O	358	O—Cl	203			C=N	615
C—F	485	O—I	234	Si—Si	340		
C—Cl	339			Si—H	393		
C—Br	276	F—F	154	Si—C	360		
C—I	240	F—Cl	253	Si—O	452		
C—S	259	F—Br	237				
		Cl—Cl	239				
		Cl—Br	218				
		Br—Br	193				

*C=O(CO_2) = 799

$$\Delta H = \underbrace{\Sigma D(\text{bonds broken})}_{\text{Energy required}} - \underbrace{\Sigma D(\text{bonds formed})}_{\text{Energy released}}$$

D represents the bond energy per mole of bonds and <u>D always has a positive sign</u>.

Example: $H_{2(g)} + F_{2(g)} \rightarrow 2\,HF_{(g)}$

$$\Delta H = \left[D_{H-H} + D_{F-F}\right] - 2D_{H-F}$$

$$= \left[1\text{mol} \times \frac{432kJ}{\text{mol}} + 1\text{mol} \times \frac{154kJ}{\text{mol}}\right] - 2\text{mol} \times \frac{565kJ}{\text{mol}}$$

$$= -544kJ$$

Enthalpy of Reaction Involving Salts

Calculate the enthalpy of the following reaction:

$$Ba(s) + Cl_{2(g)} \rightarrow BaCl_{2(s)}$$

Energy Data	
Lattice Energy	-2056 kJ/mol
1^{st} Ionization Energy of Ba	+503 kJ/mol
2^{nd} Ionization Energy of Ba	+965 kJ/mol
Electron Affinity of Cl	-349 kJ/mol
Bond Energy of Cl_2	+239 kJ/mol
Enthalpy of Sublimation of Ba	+178 kJ/mol

Solve using a Hess's Law approach:

$Ba(s) \rightarrow Ba(g)$	$\Delta H = 178$ kJ	(Sublimation)
$Ba(g) \rightarrow Ba^{+}(g) + 1\ e^{-}$	$\Delta H = 503$ kJ	(IE_1)
$Ba^{+}(g) \rightarrow Ba^{+2}(g) + 1\ e^{-}$	$\Delta H = 965$ kJ	(IE_2)
$Cl_2(g) \rightarrow 2Cl(g)$	$\Delta H = 239$ kJ	(BE)
$2Cl(g)+2e^{-} \rightarrow 2Cl^{-}(g)$	$\Delta H = 2(-349)$ kJ	(EA)
$Ba^{+2}(g)+2Cl^{-}(g) \rightarrow BaCl_2(s)$	$\Delta H = -2056$ kJ	(LE)

$Ba(s) + Cl_2(g) \rightarrow BaCl_2(s)$ $\quad \Delta H^{\circ}_f = -869$ kJ/mol