

Covalent Bond Energies and Chemical Reactions

- Consider the stepwise decomposition of methane:
 - $\text{CH}_4(\text{g}) \rightarrow \text{CH}_3(\text{g}) + \text{H}(\text{g})$ energy required: 435 kJ/mol
 - $\text{CH}_3(\text{g}) \rightarrow \text{CH}_2(\text{g}) + \text{H}(\text{g})$ energy required: 453 kJ/mol
 - $\text{CH}_2(\text{g}) \rightarrow \text{CH}(\text{g}) + \text{H}(\text{g})$ energy required: 425 kJ/mol
 - $\text{CH}(\text{g}) \rightarrow \text{C}(\text{g}) + \text{H}(\text{g})$ energy required: 339 kJ/mol
 - Total = $1652 \div 4 = 413$ kJ/mol
 - Note that the C—H bond is somewhat sensitive to its environment
- Consider the following molecules and the measured C—H bond energy (kJ/mol)

Molecule	Measure C-H bond energy (kJ/mol)
HCBBr_3	380
HCCl_3	380
HCF_3	430
C_2H_6	410

- Again, C—H bond strength varies significantly with its environment, but the concept of an average bond energy is helpful to chemists.
- The average bond energies for various types of bonds are listed below.

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	S—H	347	C=O*	745
H—I	295	N—Br	243	S—F	327	C≡O	1072
		N—O	201	S—Cl	253	N=O	607
C—H	413	O—H	467	S—Br	218	N=N	418
C—C	347	O—O	146	S—S	266	N≡N	941
C—N	305	O—F	190			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				

- In a single bond, one pair of electrons is shared, in a double bond, two pairs of electrons are shared and in a triple bond, three pairs of electrons are shared. Single bonds are the longest and weakest of the bonds. Triple bonds are the shortest and the strongest of the bonds.
- For bonds to be broken, energy must be added to a system – an endothermic process.
- Energy is released when a bond is formed.
- $\Delta H = \Sigma D(\text{bonds broken}) - \Sigma D(\text{bonds formed})$, Σ represents the sum of terms and D represents the bond energy per mole of bonds

*C=O(CO₂) = 799

- Example: Using the bond energies from above, calculate the ΔH for the reaction of methane with chlorine and fluorine to give Freon-12 (CF_2Cl_2)
 - $\text{CH}_4(\text{g}) + 2\text{Cl}_2(\text{g}) + 2\text{F}_2(\text{g}) \rightarrow \text{CF}_2\text{Cl}_2(\text{g}) + 2\text{HF}(\text{g}) + 2\text{HCl}(\text{g})$
 - Bonds broken:
 - C—H: $4 \times 413 = 1652 \text{ kJ}$
 - Cl—Cl: $2 \times 239 = 478 \text{ kJ}$
 - F—F: $2 \times 154 \text{ kJ} = 308 \text{ kJ}$
 - Total = 2438 kJ
 - Bonds formed:
 - C—F: $2 \times 485 = 970 \text{ kJ}$
 - C—Cl: $2 \times 339 = 678 \text{ kJ}$
 - H—F: $2 \times 565 = 1130 \text{ kJ}$
 - H—Cl: $2 \times 427 = 854 \text{ kJ}$
 - Total energy released = 3632 kJ
 - $\Delta H = \Sigma D(\text{bonds broken}) - \Sigma D(\text{bonds formed})$
 - $\Delta H = 2438 \text{ kJ} - 3632 \text{ kJ} = -1194 \text{ kJ}$

Homework: Calculate the ΔH for each reaction below:

1. $\text{N}_2(\text{g}) + 3\text{H}_2(\text{g}) \rightarrow 2\text{NH}_3(\text{g})$

2. $\text{CH}_4(\text{g}) + 2\text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) + 2\text{H}_2\text{O}$

3. $\text{CO}(\text{g}) + 2\text{H}_2(\text{g}) \rightarrow \text{CH}_3\text{OH}(\text{l})$

4. $\text{C}_2\text{H}_5\text{Cl}(\text{g}) + \text{Cl}_2(\text{g}) \rightarrow \text{C}_2\text{H}_4\text{Cl}_2(\text{g}) + \text{HCl}(\text{g})$

5. $\text{Cl}_2(\text{g}) + 3\text{F}_2(\text{g}) \rightarrow 2\text{ClF}_3(\text{g})$