Reactivity:



Reactants or starting material (S.M.): C_5H_{12} and O_2 Products: CO_2 and H_2O

 $\Delta E = \Delta G$: Gibbs free energy (enthalpy) change for the reaction

- This reaction is an exothermic reaction, heat is released during reaction
- ΔG = Negative for an exothermic reaction.
- E_A = Activation energy: minimum amount of energy required to activate molecules or atoms to be able to undergo a chemical reaction.
- Activated complex or transition state (T.S): Highest energy point in a reaction pathway in which bonds are being formed and broken simultaneously. A T.S. cannot be observed or isolated. Should not be confused with and an intermediate.

Thermodynamic of a chemical reaction:



 K_{eq} = equilibrium constant = [C][D] [C] = concentration of compound C [A][B]

Endothermic Reaction: Positive ΔG .



Reaction Coordinate

Reaction proceeding through an intermediate



NB: The Rate Determining Step is the TS with the larger E_A , which will be the slowest step; that is for the diagram to the left, the first step is the rate determining step.

Review

Change in Entropy $\Delta G = \Delta H - T\Delta S$ (2nd law of thermodynamics) \downarrow Change in enthalpy = bond energy

Exothermic $\Delta G = Negative$

Endothermic $\Delta G = Positive$

Bond Energy

Bond	Bond Energy (kcal/mol)
H-C	99
H-O	111
C-C	83
C=O	179
0=0	119

e.g.)
$$CH_4 + 2 O_2 \xrightarrow{\Delta} CO_2 + 2 H_2O - Exothermic reaction (releases Energy (E))$$

 $\Delta E_{reaction} = \Delta E_{SM} - \Delta E_{pdt}$

For CH ₄ :	4 x 0 2 x 0 ΔE _S	C-H bor О=О м	$ds = 4 \times 99$ = 2 x 119	= 396 kcal/mol = <u>238 kcal/mol</u> = 634 kcal/mol	ΔE_{SM} = sum of bonds broken (enthalpy)	
For product	ts:	2 C=C 4 H-O	$0 = 2 \times 179 = 2$ = 4 x 111 = 2	358 kcal/mol 444 kcal/mol	ΔE_{pdt} = sum of bonds formed	1

 $\Delta E_{reaction} = 634 \text{ kcal/mol} - 802 \text{ kcal/mol} = -168 \text{ kcal/mol}$ (exothermic reaction, energy released)

= 802 kcal/mol

Acids and Bases

Bronsted – Lowry :

- An acid donates proton (H⁺)

 ΔE_{pdt}

- A base accepts a proton (H⁺)

HCI \longrightarrow H⁺ + CI⁻ NaOH \longrightarrow Na⁺ + OH⁻

HCI + NaOH → NaCI + H-OH

• Very fast reaction as HCl is a strong acid and NaOH is a strong base. NaCl is a weak base (weak conjugate base) and H₂O is a weak acid (weak conjugate acid).

Lewis Acid/Base:

- An acid accepts a pair of electrons
- A base donates a pair of electrons

Examples of Lewis acids:

H⁺ AlCl₃ BH₃ FeCl₃

• Every Bronsted-Lowry acid/base is also a Lewis acid/ base. The converse statement is not true; not all Lewis acid/base can be classified as a Bronsted-Lowry acid/base.

$$H \xrightarrow{\frown} A$$
 $H^{\oplus} + \stackrel{\bigcirc}{:} A$ $K_{eq} = K_a = [H^+][A^-]$ $K_a = acidity constant$
[HA] $pK_a = -logK_a$

Ex #1) Methane:

$$H-CH_3 \longrightarrow H^+ + CH_3^-$$

$$K_a = [\underline{H}^+][\underline{CH}_3] = 10^{-46}$$

[HCH₃]

$$pK_a = -logK_a = 46$$

Ex # 2) Ammonia Gas:

$$H-NH_2 \longrightarrow H + \stackrel{\bigcirc}{N}H_2 \qquad K_a = \underbrace{[H^+][NH_2]}_{[NH_3]} = 10^{-36}$$

$$pK_a = 36$$

• Ammonia gas is a better acid compared to methane (bigger K_A), because nitrogen is more electronegative than carbon. It can hold a negative charge easier than carbon.

"pKa of Ammonia" in biological system

$$\begin{array}{c} H \\ H - \overset{H}{\overset{H}{\overset{}_{\oplus}}} H \xrightarrow{} & \vdots \overset{H}{\overset{}_{N}} - H & + & H^{\oplus} \\ \overset{H}{\overset{H}{\overset{}_{H}}} & \overset{H}{\overset{H}{\overset{}_{H}}} H & & H^{\oplus} \end{array}$$
Ammonium Cation $pK_{a} = 9.3$

Ex #3) Water:

H-O-H
$$\longrightarrow$$
 H + \bigcirc H + \bigcirc $K_a = [H^+][^{-}OH] = 10^{-15.7}$
[HOH]

$$pK_a = -logK_a = 15.7$$