CHEM 261 September 14, 2020

**Reactivity/ Reactions**

 **Exothermic Reaction:** Negative ∆G

Example: Combustion of Pentane





Progress of reaction is also called **Reaction Coordinate**

S.M. = starting material or reactants (e.g. pentane, oxygen)

Energy diagram for the reaction:

**NB:** ∆E = ∆G: Gibbs free energy (total) change for the reaction

G

 **Reaction coordinate** => progress of reaction

- The above reaction is an exothermic reaction, heat is released during reaction

- ∆G will be negative (∆G <0) for an exothermic (heat releasing) reaction, but will be positive (∆G >0) for endothermic reaction.

- EA= 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:**

Temperature in oK (oK = oC + 273)

 ∆G = ∆H - T∆S (2nd law of thermodynamics)

Change in enthalpy = bond energy

Change in entropy

= measure of disorder in system

∆G = -RT ln Keq

R = Gas constant = 0.082 L·atm

 mol·K

T = Temperature in oK

∆G = Change in energy of system (determines equilibrium)

Ea = Activation energy 🡪 determines rate of reaction

Keq = equilibrium constant = [C][D] [C] = concentration of compound C

 [A][B]

∆G determines product concentrations at equilibrium

Ea determines rate of reaction

**Reaction proceeding through an intermediate**

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**Endothermic Reaction**: Positive ∆G



**Summary:**

∆E = ∆G: Gibbs free energy (total) change for the reaction

Change in Entropy

∆G = ∆H - T∆S (2nd law of thermodynamics)

Change in enthalpy = bond energy

Exothermic reactions have ∆G = Negative

Endothermic reactions have ∆G = Positive

TS = Transition State: Point where bonds are partially broken and partially formed

Intermediate: Short lived species

**Bond Energy**

Radicals

Example:



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

e.g.) CH4 + 2 O2 CO2 + 2 H2O – Exothermic reaction (releases Energy (E))

∆

∆Ereaction = ∆ESM - ∆Epdt

 For CH4:

∆ESM = sum of bonds broken (enthalpy)

4 x C-H bonds = 4 x 99 = 396 kcal/mol

2 x O=O = 2 x 119 = 238 kcal/mol

∆ESM = 634 kcal/mol

∆Epdt = sum of bonds formed

2 C=O = 2 x 179 = 358 kcal/mol

4 H-O = 4 x 111 = 444 kcal/mol

∆Epdt = 802 kcal/mol

 For products:

∆Ereaction = 634 kcal/mol – 802 kcal/mol = -168 kcal/mol (exothermic reaction, energy released)