CH3104: Organic Chemistry II (Physical Organic Chemistry)

Syllabus:

- Structure and Bonding in Organic Compound and their Consequence in Reactivity. (12 lectures)
- Kinetics, thermodynamics and selectivity. (8 lectures)
- Solvent and solution properties: Empirical scale of solvent effects. (3 lectures)
- Acid - Base catalysis. (3 lectures)
- Investigation of organic reaction mechanism. (5 lectures)
- Photochemistry and Pericyclic Reaction: (9 Lectures)

Books:

Ian Fleming *Molecular Orbitals and Organic Chemical Reactions*
F. A. Carey and R. J. Sundberg *Advance Organic Chemistry, Part A: Structure and Mechanisms*
Clayden, Greeves, Warren *Organic Chemistry*
Ansyln, Dougherty, *Modern Physical Organic Chemistry*

Grading:* Endsem (complete syllabus)
Midsem
Quiz
Assignments

Molecular Interactions: Steric + Electronics

Elimination vs Substitution reaction:

Molecular Interactions: Steric + Electronics

In modern form,[3] the Klopman-Salem equation is commonly given as

$$\Delta E = \textbf{Sterics} + \text{Electronics}$$

$$= -\sum_{ab}(q_a + q_b)\beta_{ab}S_{ab} + \sum_{k<l}\frac{Q_k Q_l}{\varepsilon R_{kl}} + \sum_{r}^{occ.}\sum_{s}^{unocc.} - \sum_{s}^{occ.}\sum_{r}^{unocc.}\frac{2(\Sigma_{ab}c_{ra}c_{sb}\beta_{ab})^2}{E_r - E_s}$$

Molecular Orbitals – Frontier Molecular Orbitals (FMOs)

$$\text{Orbital interaction} = \sum\sum \frac{\sum(C_{Nu}C_{El}\beta)^2}{(EEl - ENu)}$$

Arrow pushing mechanism

- What does the curved arrows represents?

Frontier Molecular Orbitals (FMOs)

Orbital overlap b/w
HOMO and LUMO

Review FMO Theory

Salem Klopman Equation

$$\Delta E = \underbrace{-\sum_{ab}(q_a + q_b)\beta_{ab}S_{ab}}_{} + \underbrace{\sum_{k<l}\frac{Q_k Q_l}{\varepsilon R_{kl}}}_{} + \underbrace{\sum_{r}^{occ.}\sum_{s}^{unocc.} - \sum_{s}^{occ.}\sum_{r}^{unocc.}\frac{2(\Sigma_{ab}c_{ra}c_{sb}\beta_{ab})^2}{E_r - E_s}}_{}$$

Symmetry: Orbital overlap

Correct symmetry is required for effective overlap. Graphically, like phases lead to constructive interactions, but unlike phases lead to destructive interactions.