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[Gibbs Duhem Margules Equation Pd]

CH 7212: ORGANIC CHEMISTRY – I 60 Hours

1. STRUCTURE & REACTIVITY 6 hrs

Resonance, field effects, hyperconjugation, steric effects, steric inhibition of resonance.
Quantitative treatment of field and resonance effects – Hammett and Taft treatments.

2. REACTION MECHANISMS 9 hrs

Basic concepts: Thermodynamics and kinetics of reactions, Thermodynamic vs. kinetic control, Hammond postulate, microscopic reversibility, Marcus theory, Curtin – Hammett principle.
Reactive intermediates: Carbocations, carbanions, carbon free radicals, carbenes and nitrenes – generation, structure and stability.
Methods of determining mechanisms: Characterization of intermediates, kinetics, stereochemistry, kinetic isotopic effects, isotopic labeling experiments, catalysis and solvent effects.

3. STEREOCHEMISTRY 17 hrs

Molecules with 2 and 3 stereocenters – Interconversion of perspective, Fischer, sawhorse and Newman structures. R-S and E-Z notation, erythro/threo nomenclature, configuration nomenclature of molecules with 3 chiral centers, mesocompounds, systems with pseudoasymmetric centers. In-out isomerism. Classification of racemic modifications.
Axial chirality – allenes, spiranes, biphenyls – R, S notation of these systems. Planar chirality – ansa compounds, cyclophanes. Helicity – helicenes, end substituted benzphenanthrenes. Topicity, prochirality.
Conformations of substituted ethanes and substituted cyclohexanes.
Fused rings and bridged rings – decalins, nomenclature of bridged systems, norbornanes, bicyclo [2.2.2] octane.
Effect of conformation on physical and chemical properties – acyclic and cyclic compounds.

4. ALIPHATIC NUCLEOPHILIC SUBSTITUTION 11 hrs

Substitution at sp^3 carbon atom – limiting cases, S_N1 and S_N2 mechanisms. Factors influencing S_N1 and S_N2 reactions – substrate, leaving group, nucleophile and solvent effects, ambident substrates and nucleophiles – regioselectivity. Borderline cases: intermediate mechanism, mixed S_N1 and S_N2 mechanism. Neighboring group participation, non-classical carbocations. S_Ni mechanism. Allylic rearrangements.
Substitution at a trigonal carbon atom – the tetrahedral mechanism, formation of acid derivatives, cleavage of esters and N-acylation reactions. Susbtitution at vinyl carbon - tetrahedral and addition-elimination mechanisms.

5. ELIMINATION REACTIONS 6 hrs

The E2, E1, E1cB and E2C mechanisms and the spectrum of elimination mechanisms. Regioselectivity and stereochemistry of E2 and E1 reactions; effect of substrate structure, base,

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