Fundamentals of organic chemistry notes pdf

Organic chemistry carbon has unique chemistry bonds to every other element bonds to itself in long chains organic chemistry involves enormous variety many possible structures many possible reactions Organic chemists what do organic chemists do? understanding structures, reactions correlation of structures with properties synthesis of compounds with specific properties who else needs organic? basis of all life processes - the great variety of structures and reactions make life possible How to handle variety nomenclature - clear methods for naming structures and reactions structures - organized by functional groups reactions - organized by reaction types (what happens?) reactions - organized by reaction mechanisms (how does it happen?) What should you get out of organic chemistry? from complex names, be able to derive a structure from complex structures, be able to identify functional groups, predict characteristic properties work through reaction mechanisms - what is a molecule likely to do under certain conditions "think like a molecule" A reaction example CH3OH + HCl --> CH3Cl + H2O Reaction type Reaction mechanism how does the reaction occur ? (step-by-step) Bonding and Structure The Periodic Table atomic number (defines element) atomic weight (isotopes) electron shells (rows) groups (similar properties) filled shells (the noble gases) valence electrons (for bonding) Bonding - Lewis structures the octet rule ionic bonding covalent bonding - most common bonding in organic compounds Typical valence - neutral atoms in normal bonding patterns H has 1 valence electron - makes 1 bond C has 4 valence electrons - makes 4 bonds N has 5 valence electrons - makes 3 bonds + 1 lone pair O has 6 valence electrons - makes 2 bonds + 2 lone pairs F has 7 valence electrons - makes 1 bond + 3 lone pairs Recognize the appearance of these common atoms in correct structures Also recognize the common charged forms: Atom Bonds Lone Pairs Charge H 1 0 0 H+ 0 0 +1 H- 0 1 -1 C 4 0 0 C+ 3 0 +1 C. 3 1 e- 0 C- 3 1 -1 N 3 1 0 N+ 4 0 +1 N- 2 2 -1 O 2 2 0 O- 1 3 -1 O+ 3 1 +1 F 1 3 0 F- 0 4 -1 Writing organic structures Lewis structures - all electrons shown Kekule structures - show bonds as lines - lone pairs sometimes omitted condensed structures - common groups are abbreviated (e.g., CH3CH2) line structures - omit lone pairs - omit hydrogens on carbons - omit carbons (assumed to be at the end of every bond) 3-Dimensional structures dotted-line / wedge ball-and-stick space-filling Visualizing chemical structures Name (common or systematic) Condensed Formula (as usually typed out) Lewis Structure (all atoms and bonds shown) Line Structure (omit hydrogens, assume carbons at vertices) 3-D Structure (show bond orientations) Ball-and-Stick Structure (like a molecular model you could make) Space-Filling Model (approximates full size of electron distribution) methane: CH4 benzene: C6H6 penicillin: Try a 3-D image: 1) Click at the bottom after you read these instructions 2) Cross your eyes to see two double images 3) Make the middle images merge Try it! Your textbook includes a stereoviewer to make this process easier. Atomic orbitals wavefunctions - describe location of electrons s orbital (spherical) p orbitals (three: x,y,z) - (dumbbell shape - 2 lobes) d orbitals (4 lobes) - not usually needed for organic chemistry hybrid orbitals - combination orbitals Bonding attraction between negative electrons and positive nuclei - repulsions between electrons - repulsions between nuclei bonding is a balance between the attractions and repulsions characteristic bond lengths and strengths Molecular orbitals overlap of atomic orbitals electrons are close to two nuclei bonding and antibonding combinations Hybrid orbitals sp hybrids (one s plus one p) - makes two identical orbitals (linear) sp2 hybrids (one s plus two p) - makes three identical orbitals (trigonal) sp3 hybrids (one s plus three p) - makes four identical orbitals (tetrahedral) Why hybrid orbitals? good shape (directional) allows high overlap in bonding maximizes electron density between atoms good orientation minimizes repulsions between orbitals Identifying the hybridization of carbon identify sigma and pi bonds around the carbon atom (you need one sigma bond for each neighboring atom and you need a total of four bonds for carbon) Neighboring Atoms Sigma Bonds Pi Bonds Hybrid Structure 4 4 0 sp3 tetrahedral 3 3 1 sp2 trigonal planar 2 2 2 sp linear Molecular geometry by VSEPR electron pairs repel one another, maximize their separation Electronegativity tendency of an atom to attract electrons in a covalent bond in the Periodic Table, electronegativity increases to the right and up F > O > Cl ~ N > Br > C > H > metals Polar covalent bonds electrons in a covalent bond may not be equally shared H-Cl is polarized with excess electron density closer to Cl Polar bonds to carbon C-C bonds are nonpolar C-H bonds are generally considered nonpolar C-X bonds are polarized with carbon partially + for X = F, Cl, Br, I, O, S, N C-M bonds are polarized with carbon partially - for M = metals Functional Groups a specific arrangement of atoms define chemical families determine chemical properties basis of nomenclature organization of textbooks examples - the simple oxygen families: alcohols, ethers, aldehydes, ketones, carboxylic acids Resonance more than one possible Lewis structure for a compound What's the best Lewis structure? follow the octet rule electronegativity determines the best place to locate charges carbon monoxide (CO) nitromethane (CH3NO2) Electron-pushing keeping track of electrons is crucial in organic chemistry curved electron arrows indicate electron pair movement - in converting resonance forms, or later, in reactions Introduction Organic Chemistry: Field of chemistry which studies carbon-based compounds Homologous Series: A series of compounds of the same family, with the same general formula, which differ from each other by a common structural unit. Hydrocarbons: Alkanes: CnH2n+2 Alkyl: CnH2n+1 (Hydrogen of CH4 replaced with other group) Alkenes: CnH2n Alkynes: CnH2n-2 Functional Groups Alcohols: CnH2n+1OH Aldehydes: CnH2nO Ketones: CnH2nO Halogenoalkanes: CnH2n+1X Homologous series which contain functional groups also have similar physical and chemical properties within the series. Most of the time its reactive and contains oxygen or nitrogen. In alkene and alkyne, the double and triple bonds are functional groups. Physical properties of homologous series Generally, as the length of the chain increases, the boiling point increases (due to increased SA, greater chance of intermolecular bonding, more energy to break bonds, higher boiling point) Chemical formulae of organic compounds Lewis dot structures: Useful to visualize valence electrons Empirical formula: Simplest ratio of atoms in a molecule Molecular formula: Actual number of atoms present in molecule Structural formula: Takes into account the possible structure Full structural formula: 2D representations showing all atoms and bonds and their positions Condensed structural formula: All atoms and relative positions, bonds are omitted Skeletal formula: Carbon and hydrogen atoms are not shown, end of each line and vertex represents C atom. Functional groups shown as well. Nomenclature (Naming) IUPAC is the world authority in naming and the one used by IB Best way to learn this is to practice naming multiple compounds Identify the longest chain and thus the root name. 1 carbon = meth- 2 carbon = eth- 3 carbon = prop- 4 carbon = but- 5 carbon = pent- 6 carbon = hex- 7 carbon = hept- 8 carbon = oct- Identify the type of bonding in chain or ring All single bonds = -an- One double bond = -en- One triple bond = -yn- Identify functional or alkyl groups (this may by at beginning or end of name) Alkane: only hydrogen joined to chain -e Hydroxyl: -ol Amine: amino- Amide: -amide Nitrile: -nitrile Halo: chloro-, bromo- or iodo- Aldehyde: -al Ketone: -one Carboxyl: -oic acid Ether: -oxy- Ester: -oate Use numbers to give position of groups or bonds along chain. Always aim to have lowest numbers. Structural isomer Compounds with same chemical formula but a different structural formula. Have unique physical and chemical properties Saturated and unsaturated hydrocarbons Saturated: All carbon to carbon bonds are single bonds (Saturated with H atoms) Unsaturated: Contain double or triple bonds Functional groups When naming, the position of group is identified by giving the number of the carbon atom to which it is attached When numbering, functional groups take priority over substituents and c-c multiple bonds Classifying molecules: primary, secondary, and tertiary compounds These are three classes of compounds Primary (1°): Carbon atom bonded to functional group is also bonded to one other carbon atom Secondary (2°): Carbon atom bonded to functional group is also bonded to two other carbon atoms Tertiary (3°): Carbon atom bonded to functional group is also bonded to three other carbon atoms Classifying halogenoalkanes Alkanes undergo free-radical substitution reactions with halogens Whether primary, secondary or tertiary depends on conditions and mechanism of reaction Classifying alcohols Position of the hydroxyl (OH) group determines the class of alcohol Classifying amines Classified depending on number of alkyl groups bonded to the nitrogen atom of functional group N signifies the substituent on the amine. Refer to examples to understand. Aromatic hydrocarbons Aromatic hydrocarbons are characterized by the presence of benzene Benzene is C6H6 composed of alternating double and single bonds Benzene contains 6 sp2 hybridized carbon atoms bonded to one another, and each carbon bonded to single hydrogen The p orbital overlaps creating a continuous π bond above and below plane of carbon atoms Benzene has a resonance structure

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