

Organic Chemistry

Paula Yurkanis Bruice, 5th Edition

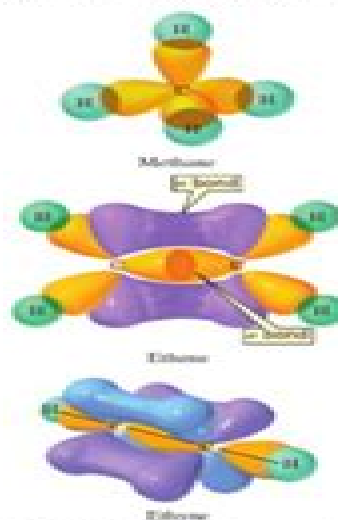
Prepared by Matthew B. Anderson

Chapter 1 Electronic Structure and Bonding • Acids and Bases

1. Atoms consist of protons (p^+), neutrons (n), and electrons (e^-). **Atomic number** is the number of p^+ ; **mass number** is the sum of p^+ and n . **Isotopes** have the same number of p^+ with different numbers of n . The **atomic weight** of an element is the average weighted mass of its atoms (1.1).
2. An **atomic orbital** (s , p , d , f) is the volume of space around a nucleus where an electron is most likely to be found. An electron goes into the lowest energy orbital available (**aufbau principle**), with two e^- in each orbital (**Pauli exclusion principle**). An e^- will occupy an empty **degenerate** (same energy) orbital before it will pair up with another e^- (**Hund's rule**). Core e^- are in filled shells; **valence e^-** are used for bonding (1.2).
3. Atoms give up or accept e^- to achieve an outer shell of eight electrons (**octet rule**). **Electropositive** elements (on the left of the periodic table) lose e^- to form cations; **electronegative** elements (on the right) gain e^- to form anions. **Ionic bonds** are formed by electrostatic attraction between cations and anions. **Electronegativity** is a measure of an atom's ability to attract e^- . Atoms form **covalent bonds** by sharing valence e^- . **Nonpolar covalent bonds** are formed by atoms with the same electronegativity; **polar covalent bonds** are formed by atoms with different electronegativity. A polar bond has a **dipole** with a **dipole moment**, μ (debye). **Electrostatic potential maps** show how charge is distributed: red ($-$) and blue ($+$) (1.3).
4. **Lewis structures** represent compounds, showing all bonding and lone pair e^- . The **formal charge** on an atom = the number of valence e^- minus $1/2$ the bonding e^- minus the lone pair e^- . Carbocations have a positively charged carbon; carbanions have a negatively charged carbon; a carbon radical has a carbon with an unpaired e^- . **Kekulé structures** depict bonds as lines. **Condensed structures** use subscripts and few, if any, bonds (1.4).
5. An s atomic orbital is spherical; the $2p$ atomic orbital has a **radial node**. There are three degenerate, perpendicular p orbitals; each has a node at its nucleus (1.5).
6. **Bond length** is the distance between nuclei; **bond dissociation energy** is the energy required to break a bond. Two atomic orbitals combine to form two molecular orbitals, a **bonding MO** (σ or π) and an **antibonding MO** (σ^* or π^*). A **sigma (σ) bond** is

cylindrically symmetrical. Three p orbitals overlap side-to-side to form a **π bond** (1.6).

7. Methane has four identical covalent bonds formed using four **hybrid (sp^3) orbitals**, which result from mixing one $2s$ and three $2p$ atomic orbitals. It has **tetrahedral (109.5°) bond angles**. Ethane has sp^3 carbons and 109.5° bond angles. Ethene (with a **double bond**) has sp^2 carbons and 120° bond angles. Ethyne (with a **triple bond**) has sp carbons and 180° bond angles. All single bonds are σ bonds; a **double bond** consists of 1 σ bond and 1 π bond; a **triple bond** consists of 1 σ bond and 2 π bonds. The more s character, the shorter and stronger the bond and the larger the bond angle. (1.6–1.9, 1.14).



8. The O and N of water and ammonia are sp^3 hybridized; H_2O has 104.5° bond angles; NH_3 has 107.3° bond angles. C^+ and C^- are sp^2 ; $C^{\cdot-}$ is sp^3 (1.11, 1.12).
9. A **Brønsted acid** donates a proton (H^+); a **Brønsted base** accepts a proton, forming a **conjugate base** and a **conjugate acid**, respectively. The **acid dissociation constant** (K_a) is a measure of the acidity of a compound; $pK_a = -\log K_a$; the lower the pK_a , the stronger the acid. Protonated carboxylic acids and protonated alcohols = **strong acids** ($pK_a < 0$); carboxylic acids = **weak acids** ($pK_a \sim 5$); protonated amines = **very weak acids**

($pK_a \sim 10$); alcohols and water ($pK_a \sim 15$). The equilibrium constant for an acid-base reaction = (reactant K_a) / (product K_a). When atoms are the same size, the more electronegative the atom to which the hydrogen is attached, the stronger the acid. Relative electronegativities: $sp > sp^2 > sp^3$. When atoms are very different in size, the strongest acid will have its hydrogen attached to the largest atom. For example, acid strengths: $HI > HBr > HCl > HF$. The stronger the acid, the weaker its conjugate base. Weak bases are stable bases. A **Lewis acid** accepts a share in a pair of e^- ; a **Lewis base** donates a share in a pair of e^- . **Curved arrows** are used to show electron flow; the arrow begins where the electrons originate and points to where they end up (1.16–1.26).

Chapter 2 An Introduction to Organic Compounds

1. **Hydrocarbons** contain only C and H. **Alkanes** are hydrocarbons with only single bonds. **Constitutional isomers** have the same molecular formula but differ in the way the atoms are connected. **IUPAC** (systematic) and common names are used to name compounds. CH_3 = a **methylene group**. A **primary (1°) carbon** is bonded to one other C; a **secondary (2°) carbon** is bonded to 2 Cs; a **tertiary (3°) carbon** is bonded to 3 Cs. Substituents are indicated as prefixes, with the **parent hydrocarbon** numbered in the direction that puts the lowest number in the name of the compound. Substituents are listed alphabetically; di, tri, tetra, are used for identical alkyl groups, but are not alphabetized; sec and tert are also not alphabetized, but iso and cyclo are. In a **cycloalkane** with two substituents, the first cited substituent gets the lower number (2.1–2.3).



2. **Alkyl halides** and **ethers** are named as substituted alkanes; **alcohols** and **amines** are named using a functional group suffix. Substituents on the nitrogen are preceded by an N. If a parent chain has a substituent, the substituent gets the lowest number; if it has a functional group, the functional group gets the lowest number; if it has both a substituent and a functional group, the functional group gets the lowest number. Only if the functional group gets the same number in either direction, is the

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David R. Klein



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Reaction Mechanisms in Organic Chemistry Metin Balci, 2021-12-01 An accessible and step by step exploration of organic reaction mechanisms In *Reaction Mechanisms in Organic Chemistry* eminent researcher Dr Metin Balci delivers an excellent textbook for understanding organic reaction mechanisms The book offers a way for undergraduate and graduate students to understand rather than memorize the principles of reaction mechanisms It includes the most important reaction types including substitution elimination addition pericyclic and C C coupling reactions Each chapter contains problems and accompanying solutions that cover central concepts in organic chemistry Students will learn to understand the foundational nature of ideas like Lewis acids and bases electron density the mesomeric effect and the inductive effect via the use of detailed examples and an expansive discussion of the concept of hybridization Along with sections covering aromaticity and the chemistry of intermediates the book includes A thorough introduction to basic concepts in organic reactions including covalent bonding hybridization electrophiles and nucleophiles and inductive and mesomeric effects Comprehensive explorations of nucleophilic substitution reactions including optical activity and stereochemistry of S_N2 reactions Practical discussions of elimination reactions including halogen elimination and Hofmann elimination In depth examinations of addition reactions including the addition of water to alkenes and the epoxidation of alkenes Perfect for students of chemistry biochemistry and pharmacy *Reaction Mechanisms in Organic Chemistry* will also earn a place in the libraries of researchers and lecturers in these fields seeking a one stop resource on organic reaction mechanisms

Advanced Organic Chemistry Francis A. Carey, Richard J. Sundberg, 2006-05-02 Since its original appearance in 1977 *Advanced Organic Chemistry* has found wide use as a text providing broad coverage of the structure reactivity and synthesis of organic compounds The Fourth Edition provides updated material but continues the essential elements of the previous edition The material in Part A is organized on the basis of fundamental structural topics such as structure stereochemistry conformation and aromaticity and basic mechanistic types including nucleophilic substitution addition reactions carbonyl chemistry aromatic substitution and free radical reactions The material in Part B is organized on the basis of reaction type with emphasis on reactions of importance in laboratory synthesis As in the earlier editions the text contains extensive references to both the primary and review literature and provides examples of data and reactions that illustrate and document the generalizations While the text assumes completion of an introductory course in organic chemistry it reviews the fundamental concepts for each topic that is discussed The Fourth Edition updates certain topics that have advanced rapidly in the decade since the Third Edition was published including computational chemistry structural manifestations of aromaticity enantioselective reactions and lanthanide catalysis The two parts stand alone although there is considerable cross referencing Part A emphasizes quantitative and qualitative description of structural effects on reactivity and mechanism Part B emphasizes the most general and useful synthetic reactions The focus is on the core of organic chemistry but the information provided forms the

foundation for future study and research in medicinal and pharmaceutical chemistry biological chemistry and physical properties of organic compounds The New Revised 5th Edition will be available shortly For details click on the link in the right hand column

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