Bio-110: Exercise 1

Discussion

28.02.2025

Illustration: David S. Goodsell

Agenda

1. Nomenclature
2. Structure Representation
3. Hybridization
4. Resonance / Delocalization
5. Aromaticity

Nomenclature

Lecture Slide 36

Names for straight-chain alkanes

N	Systematic Name	Chemical formula	Rest
1	Methane	CH_4	Methyl
2	Ethane	C_2H_6	Ethyl
3	Propane	C_3H_8	Propyl
4	Butane	C_4H_{10}	Butyl
5	Pentane	C_5H_{12}	
6	Hexane	C_6H_{14}	
7	Heptane	C_7H_{16}	
8	Octane	C_8H_{18}	
9	Nonane	C_9H_{20}	
10	Decane	$C_{10}H_{22}$	
11	Undecane	$C_{11}H_{24}$	
12	Dodecane	$C_{12}H_{26}$	

Nomenclature

Lecture Slide 37

IUPAC System

Main Chain Identification

1) The largest possible number of highest-ranking characteristic groups

2) The largest possible number of C-atoms

3) The largest possible number of multiple (double- & triple) bonds

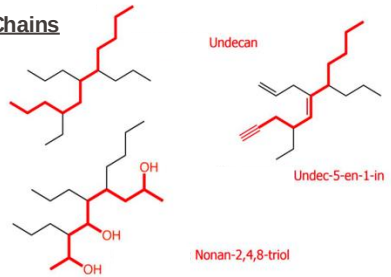
4) The largest possible number of double bonds

5) The largest possible number of side-chains

6) The chain with the lowest locants for the side chain

7) The chain with the least branched side chains

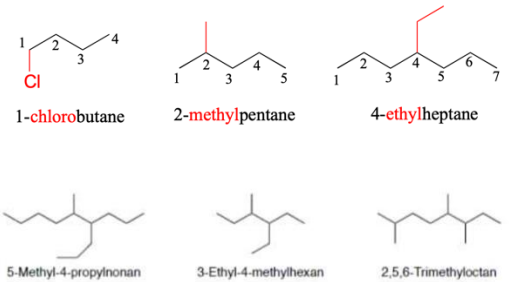
Example Main Chains



Main Chain Numbering

1) To localize the side chains, the atoms of the main chain are numbered consecutively. The numbering is chosen so that the side chains (regardless of their structure) have the lowest possible number of positions (locants). ({2,3,8} > {2,4,5})

2) If, taking this criterion into account, there are still various options for choosing the starting point of the numbering, then the lowest locant is added to the side chain listed first in the name. (Butyl > Ethyl > Methyl > ...)



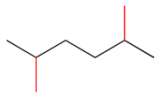
Nomenclature

Lecture Slide 38

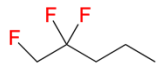
IUPAC System

Multiplicative prefixes for compound substituents

- Simple substituents, e.g. Methyl
  - di-
  - tri-
  - tetra-
  - penta-
  - hexa-
  - …

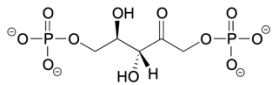


2,5-dimethylhexane



1,2,2,-trifluoropentane

- Combinend (substituted) substituents
  - bis-
  - tris-
  - …

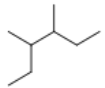
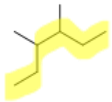
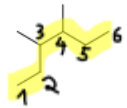
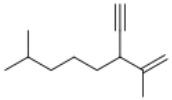
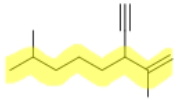
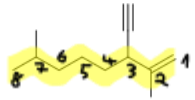
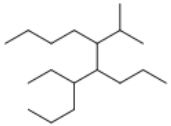
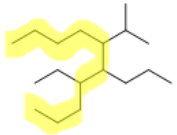
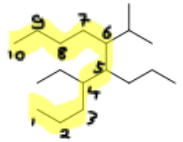
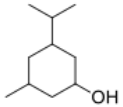
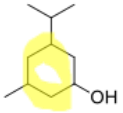
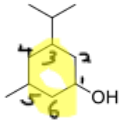


ribulose-1,5-bisphosphate

Functional Group	Suffix
Alkane	-an
Alkene	-en
Alkyne	-yne (German: -in)
Alcohols	-ol
Aldehydes	-al
Ketones	-one

Nomenclature

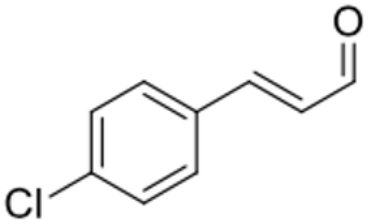
Ex. 1.3 (a)

Molecule	Main Chain	Numbered Main Chain	IPAC Name
			3,4-Dimethylhexane
			3-Ethynyl-2,7-dimethyloct-1-en
			4-Ethyl-6-(1-methylethyl) 5-propyldecan (alphabetical order, not numbers)
			5-Methyl-3-(1-methylethyl) cyclohexan-1-ol

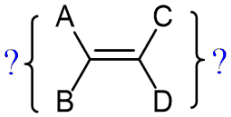
Nomenclature

Ex. 1.3 (c) (v)

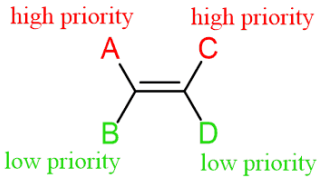
(2E)-3-(4-Chlorphenyl)prop-2-en-1-al



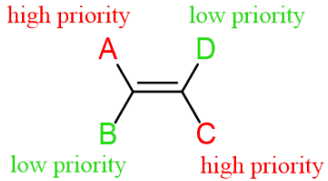
_E_ and _Z_ configuration of double bonds based on group priority

Determine priority of A and B ?  ? Determine priority of C and D

*Suppose **A is higher than B** and **C is higher than D***



It is ***Z*** if the high priority groups are on the **same side of the double bond**.



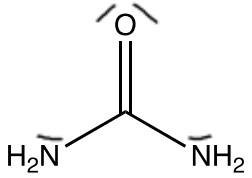
It is ***E*** if the high priority groups are on **opposite sides of the double bond**.

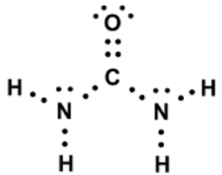
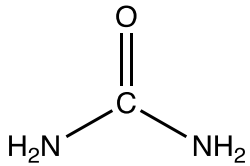
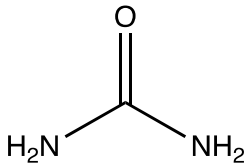
Source: https://www.chemistrysteps.com/e-and-z-alkene-configuration-practice-problems/

Structure Representation

Ex. 1.1 (i)

Suggestion to work with:



Lewis	Kekulé	Line Structure
		

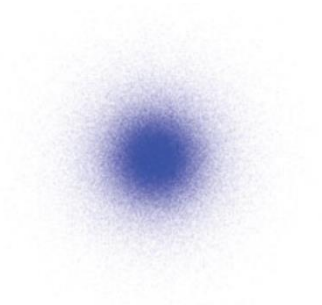
Electron representation ⟷ Level of Abstraction

But where are the electrons *really*?

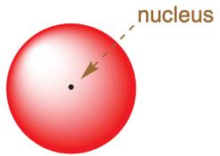
Atomic orbitals

Reading Recommendation: Clayden Chapter 4

From quantum chemistry: We have to think of **electrons** in atoms (and in molecules) as having a **probability** of being **in a certain place** at a certain time

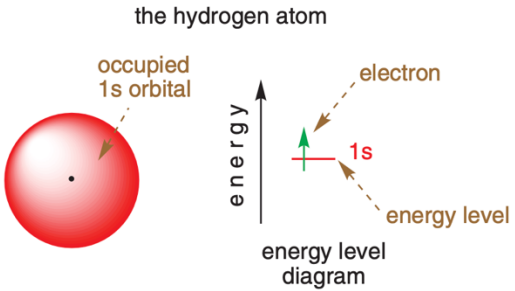


probability distribution of electron in 1s orbital

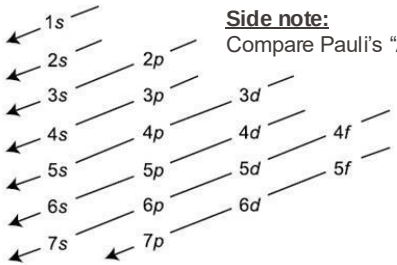


schematic diagram of 1s orbital

conventional picture of 1s orbital



energy level diagram



Side note:
Compare Pauli's "Aufbau principle"

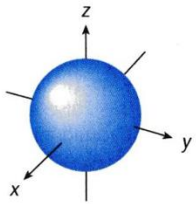
Source: Clayden Book

Atomic orbitals

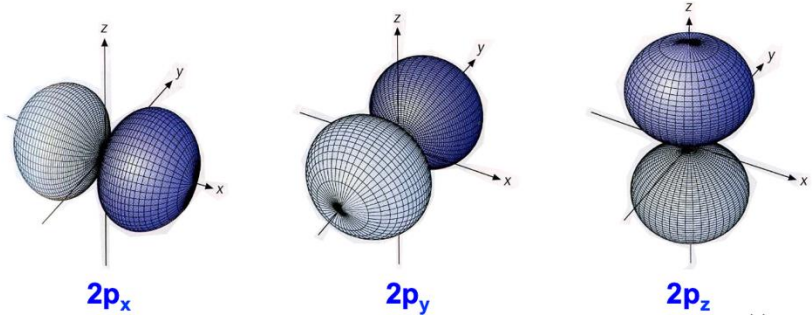
Reading Recommendation: Clayden Chapter 4

Overview over orbitals commonly relevant in Organic Chemistry

S-orbitals



P-orbitals

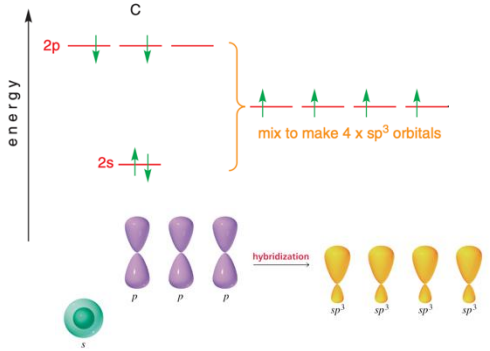


Hybridization

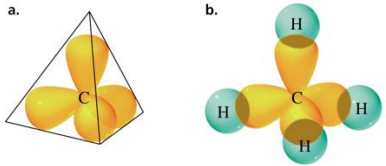
Reading Recommendation: Clayden Chapter 4

What is hybridization? Combine the 2s and 2p orbitals to make four new orbitals (that guide molecular bond geometry)

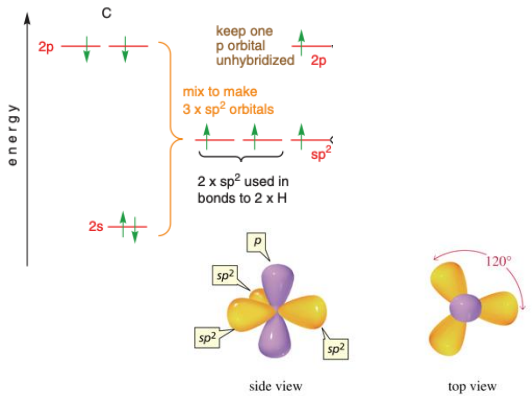
sp^3



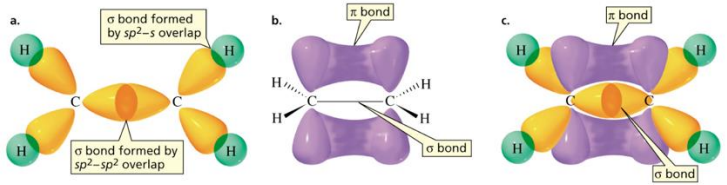
Example: Methane



sp^2



Example: Ethene



- Bond angle: 109.5° -Tetraedral
- Electron pairs as distant from each other as possible

Sources: Clayden Book; Paula Y. Bruice, Organic Chemistry (4th Ed), Prentice Hall, 2005

Hybridization

2 Simple Ways to determine hybridization (2nd period elements)

Determine Used p-orbitals

1. Start from sp^3
2. Subtract one p-orbital for each π-bond
3. Subtract one p-orbital for each empty orbital (positive charge)

Identify by means of geometry

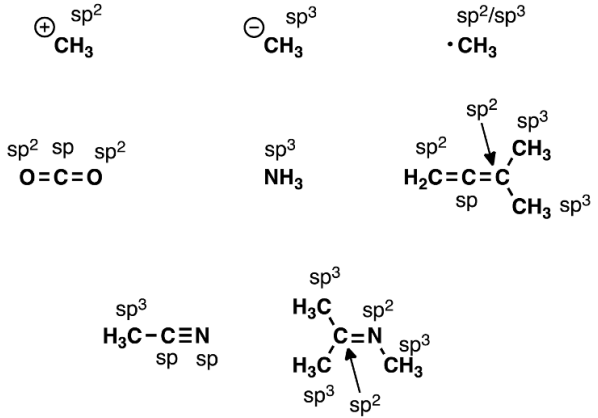
1. N = # direct bonding partners + # free electron pairs
2. Use N to determine geometry and thus hybridization:
   - N = 4 is tetrahedral → sp^3
   - N = 3 is trigonal → sp^2
   - N = 2 is liner → sp

Hybridization

Ex. 1.8 (a)

Determine Used p-orbitals

1. Start from sp^3
2. Subtract one p-orbital for each π-bond
3. Subtract one p-orbital for each empty orbital (positive charge)



Identify by means of geometry

1. N = # direct bonding partners + # free electron pairs
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   - N = 4 is tetrahedral → sp^3
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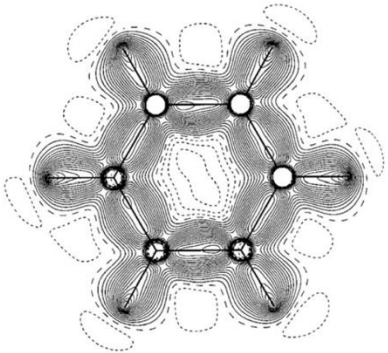
   - N = 2 is liner → sp

Resonance

Book Chapter 2.3
Clayden Chapter 7

Delocalization of electrons within molecules

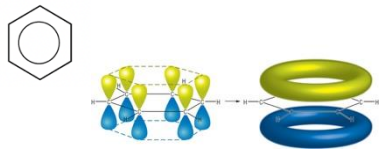
Benzene



Electron diffraction image of a molecule of benzene

Resonance Contributors

Resonance Hybrid



Formate

Resonance Contributors

Resonance Hybrid

Using Chemical Arrows:

- Cruved arrow: e⁻ movements
- Resonance arrow
- Equilibrium arrow
- Reaction arrow

Drawing Resonance Contributors

Book Chapter 2.3
Clayden Chapter 7

These are no chemical reactions! Rather, you are seeing the exact same molecule depicted in different ways

Rules for drawing resonance structures:

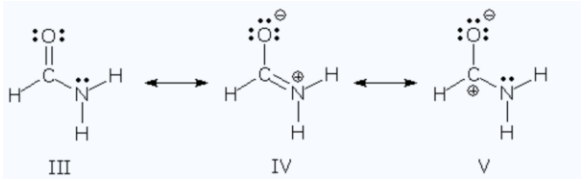
1. Resonance contributors involve the 'imaginary movement' of π-bonded electrons or of lone-pair electrons that are adjacent to (i.e. conjugated to) π bonds
2. The position of an atom within the molecule never changes (this is isomerism)
3. All resonance contributors for a molecule or ion must have the same net charge.
4. All resonance contributors must be drawn as proper Lewis structures, with correct formal charges

Criteria of relevance:

Not all resonance structures of a compound are equally relevant, i.e. some resonance structures describe the actual state of the molecule better than others. The main criterion here is the stability of the molecule if it would actually exist in the resonance structure. The more stable the molecule, the more relevant the associated resonance structure.

Example criteria (in that order):

- Octet: All atoms should have an octet to represent a relevant structure
- Charge separation: The fewer charges occur in the structure, the more relevant the resonance structure. Equal charges on neighbouring atoms are particularly unstable
- Electronegativity: Negative charges in structures with charges should be localised on electronegative atoms, and vice versa

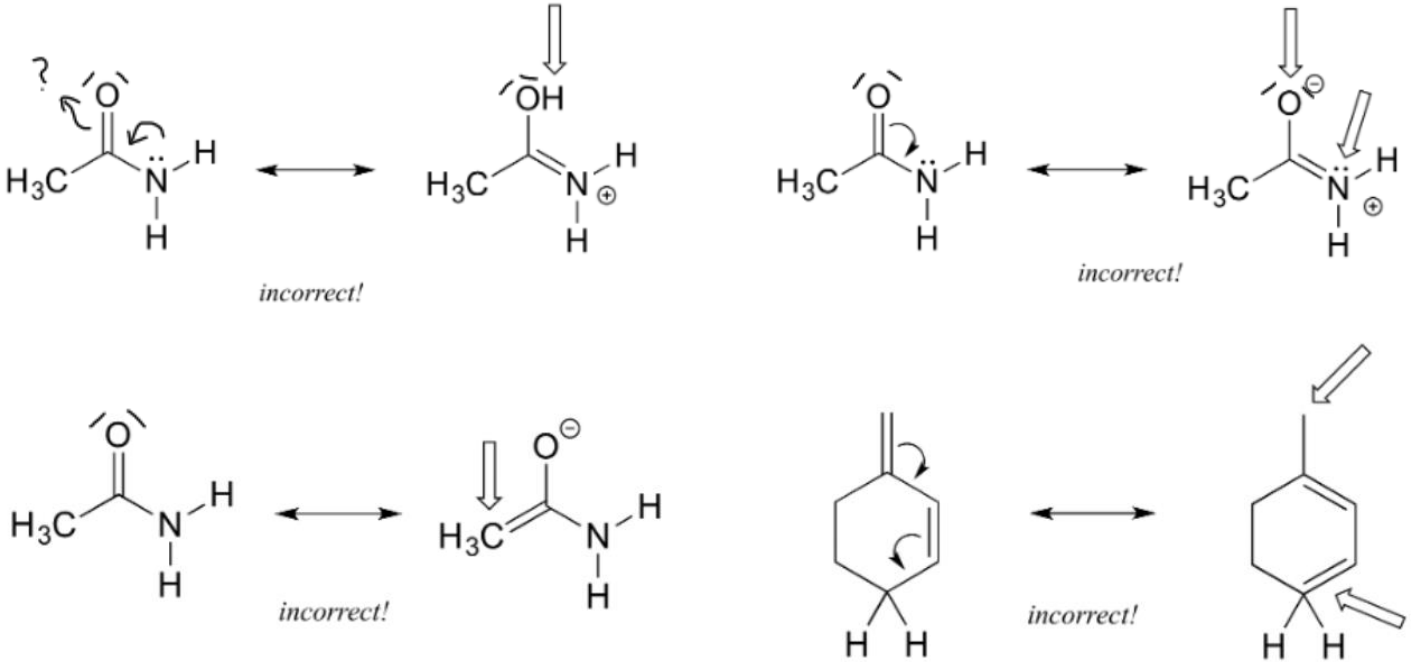


III IV V

major minor very minor

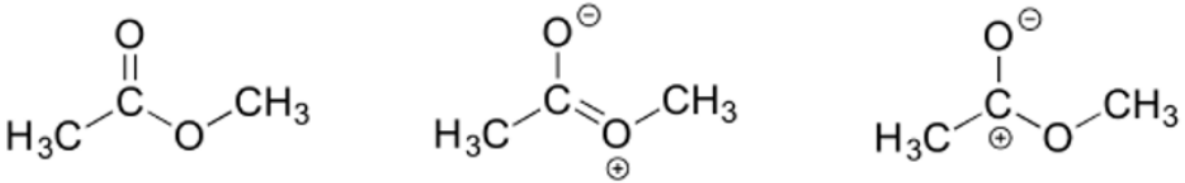
Resonance

Ex. 1.9 (a) – **Hint:** Always explicitly draw the electron lone pairs of the molecule



Resonance

Ex. 1.9 (b)



The contributor on the **left** is the most stable: there are no formal charges. The contributor in the **middle** is intermediate stability: there are formal charges, but all atoms have a complete octet. The contributor on the **right** is least stable: there are formal charges, and a carbon has an incomplete octet.

Aromaticity

Aromaticity

Re-Cap: Criteria for aromaticity

1. The molecule or group must be cyclic.
2. The ring must be planar
3. Each atom in the ring must be sp^2-hybridized
4. The number of π electrons in the ring must equal 4n+2, where n is any positive integer including 0.

Analysis:

1. All conditions satisfied → Aromatic
2. Conditions 1-3 satisfied, but 4n π electrons → Anti-Aromatic
3. Any of conditions 1-3 not satisfied → Non-Aromatic

Aromaticity

Ex. 1.7 (a)

Re-Cap: Criteria for aromaticity

1. The molecule or group must be cyclic.
2. The ring must be planar
3. Each atom in the ring must be sp^2-hybridized
4. The number of π electrons in the ring must equal 4n+2, where n is any positive integer including 0.

Analysis:

1. All conditions satisfied → Aromatic
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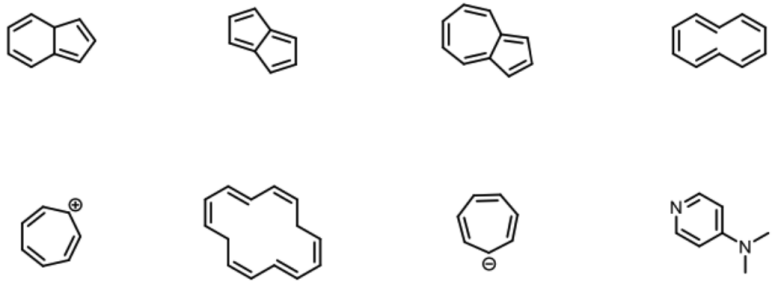

non-aromatic not-conjugated 8π electrons	**anti-aromatic 8π electrons**	**aromatic 10π electrons**	**non-aromatic not-planar 10π electrons**
aromatic 6π electrons	**non-aromatic not-conjugated 12π electrons**	**anti-aromatic 8π electrons**	**aromatic 6π electrons**