AS A REMINDER:

More examples for representation of molecules



Steroid (C₁₇)

- 1. <u>Estradiol</u> estrogen steroid hormone
 - Discovered and elucidated by Adolf Butenandt and Edward Doisy (1929)
 - 4 ton of hog ovaries \rightarrow 4 mg of estradiol
 - -



Female hormone All purple atoms are in the same plane

Types of C:

 $CH_3 - Methyl$ $CH_2 - Methylene$ CH - Methine -C - - -C - --Quaternary carbon



Functional groups in testosterone (alkene and ketone and alcohol)

Degree of unsaturation: each ring or double bond account for one degree of unsaturation, calculation of DOU will be discussed in the future lecture.

DRAWING CHEMICAL STRUCTURES



Open chain form





Bond line form

$$MF = C_4 H_8 O_3$$

- C=O is a carbonyl
- COOH is a carboxylic acid

The above compound can also be represented in the following forms, resulting from the free rotation of single bonds (sigma).



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Example:



Note: Single bonds, in general, have free rotation

Formal Charge

- Convention to keep track of charges
- \sum (sum of) of formal charges on all atoms in a molecule = overall charge on molecule

Rules for calculating formal charge

- Add number of protons in nucleus
- Subtract number of inner shell electrons
- Subtract number of unshared electrons
- Subtract ½ of the number of shared outer shell electrons

Examples:

1. NaNO₂ (sodium nitrite; food preservative) Nitrite anion



Overall charge on the nitrite anion is = -1

Single bonded oxygen: +8 (number of protons) -2 (1s electrons) -6 (unshared electrons) $\frac{1}{2} \ge 2 = -1$ (1/2 of shared electrons) -1 Central N: +7 (number of protons) -2 (1s e⁻) -2 (unshared e⁻) -3 (1/2 shared e⁻) = 0 2. Methyl radical (sp³, tetrahedral)



Overall charge on the methyl anion is = 0Very unstable since it doesn't have an inert gas configuration

- Formal Charge on Carbon +6 (number of protons) -2 (1s electrons) -1 (unshared electrons) $\frac{1}{2} \ge 6 = -3$ (1/2 of shared electrons) 0
- **3.** Methyl cation (carbocation, sp², planar)
 - (sp² hybridized carbon, planar shape)
 - can be reactive intermediate in principle

Overall charge on the methyl anion is = +1



4. Methyl anion (sp³, tetrahedral)



Overall charge on the methyl anion is = -1

Formal Charge on Carbon
+6 (number of protons)
-2 (1s electrons)
-2 (unshared electrons)
$$\frac{1}{2} \ge 6 = -3$$
 (1/2 of shared electrons)
-1

Formal Charge on Carbon +6 (number of protons) -2 (1s electrons) 0 (unshared electrons) $\frac{1}{2} \ge 6 = -3$ (1/2 of shared electrons) +1

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5. Sodium Nitrate (NaNO₃)



Resonance Structures: Different drawings (or pictures) of the same molecule made by moving electrons but not atoms

- Move the electrons, keeping the position of the atoms same -
- -Good resonance structures:
 - Maintain inert gas configuration around each atom
 - Avoid separation of charges
- Avoid like-charges on adjacent atoms
- Double headed arrow $(\leftarrow \rightarrow)$ is used indicate resonance forms Fish Hook and double headed arrows are used to show electron movement



Fish Hook Arrow Show movement of 1e⁻

Examples

1. Hydrogen gas, H₂



In the bad representations, non- inert gas configuration and extra charges have been created

2. Sodium Nitrate, NaNO₃, Na⁺ NO₃⁻ (Nitrate has 3 resonance forms shown here)



No inert gas configuration disrupted No extra charge created

- The O atoms contain partial single and double bond characteristics (each O has -2/3 charge)
- 3. Allyl Cation



-electrons are delocalized between the two carbons on both side of the central C and C atoms has -1/2 charge and contains partial double and single bond character.

4. Keto-Enol



5. Sodium Nitrite, NaNO₂



Nitrite anion is reactive in both O atoms. Electrons are delocalized in more than one atom - both O atoms has -1/2 charge and contains partial double and single bond character.

6. Allyl Radical



The radical is relatively stable due to resonance.

7. Propyne cation



8. CH₄ Methane – below are POOR resonance structures – additional charges or unshared electrons (not inert gas configuration)

• CH₃

but methyl radical – can be reactive intermediate in principle

$$\stackrel{\bigcirc}{\mathsf{CH}_3}$$
 $\stackrel{\oplus}{\mathsf{CH}_3}$



but methyl anion – can be a reactive intermediate in principle



but methyl cation – can be a reactive intermediate in principle



8. Benzene



Intermolecular Forces: (forces present between molecules)

- Attractive intermolecular forces:
 - i) **Hydrogen bonding** strongest on per atom basis (e.g. base recognition in forming DNA helix) (also in RNA)
 - Linus Pauling development of H bonding
 - ii) **Dipole-dipole interaction** (Intermediate strength)
 - iii) **London forces** (temporary dipole; hydrophobic bonding) weakest on per atom basis distortion of inner shells.

Electronegativity:

- An atom's desire for electrons (negative charge).
- On the periodic table, electronegativity increases as you go from left to right (up to inert gases, which are not electronegative) and as you go from down to up
- Halogens (F, Cl, Br, I) are highly electronegative
 - i.e. Fluorine is the most electronegative atom (wants to gain the inert gas configuration of Ne) and is small (has few electrons)

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It influences acidity of H's attached, as well as the intermolecular forces between molecules.