Lecture 2

Fundamentals and Applications (CSO201A)

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Functional Groups

A functional group is an atom or a group of atoms with characteristic chemical and physical properties.

Most organic molecules contain a carbon backbone consisting of C—C and C—H bonds to which functional groups are attached.

Structural features of a functional group include:

Heteroatoms—atoms other than carbon or hydrogen.

Bonds most commonly occur in C—C and C—O double bonds.

Functional Groups-1

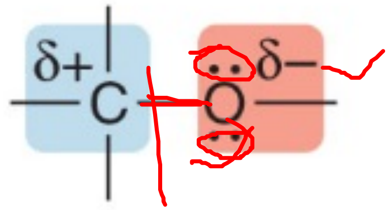
Functional groups distinguish one organic molecule from another.

They determine a molecule's:

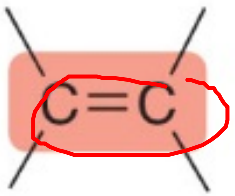
- Geometry
- Physical properties
- Reactivity

Reactivity of Functional Groups

Heteroatoms and bonds confer reactivity on a particular molecule.
Heteroatoms have lone pairs and create electron-deficient sites on carbon.
A bond makes a molecule a base and a nucleophile, and is easily broken in chemical reactions.



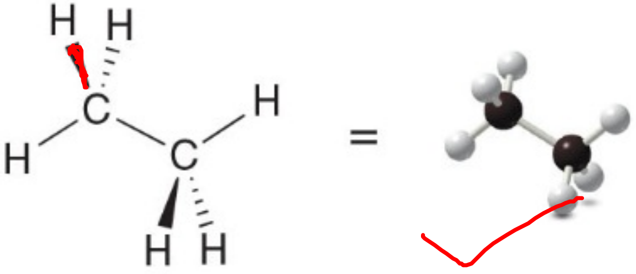
- Lone pairs make O a base and a nucleophile.
- The C atom is electron deficient, making it an electrophile.



- The π bond is easily broken.
- The π bond makes a compound a base and a nucleophile.

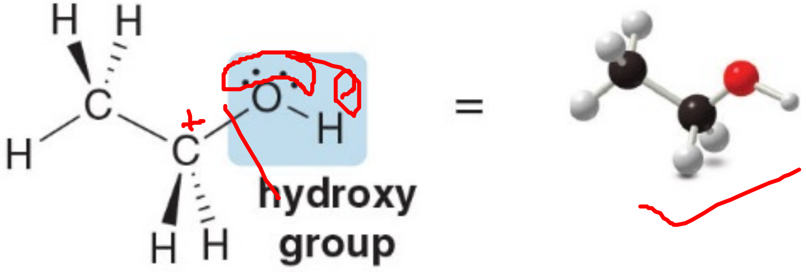
Parts of a Functional Group

carbon skeleton　　reactive part



ethane

- all C–C and C–H σ bonds
- no functional group



ethanol

- polar C–O and O–H bonds
- two lone pairs

Ethane, a Molecule with No Functional Group

This molecule has only C—C and C—H bonds.
It contains no polar bonds, lone pairs, or bonds.
Therefore, ethane has no reactive sites (functional groups).
Consequently, ethane and other alkanes are very unreactive.

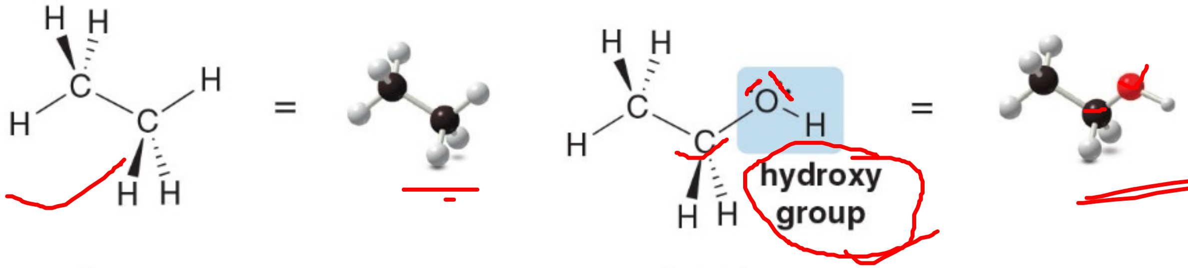
CH_3-CH_3

Ethanol

CH_3-CH_2-OH

This molecule has an OH (called a hydroxy group) attached to its backbone.
Compounds containing an OH group are called alcohols.
The hydroxy group makes the properties of ethanol very different from the properties of ethane.
Ethanol has lone pairs and polar bonds that make it reactive.
Other molecules with hydroxy groups will have similar properties to ethanol.

Ethanol-1



ethane

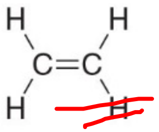
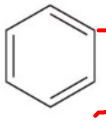
- all C–C and C–H σ bonds
- no functional group

ethanol

- polar C–O and O–H bonds
- two lone pairs

Hydrocarbons

Hydrocarbons are compounds made up of only the elements carbon and hydrogen.
They may be aliphatic (ex. alkanes, alkenes, alkynes) or aromatic.

Type of compound	General structure	Example	Functional group
Alkane	R—H	CH_3CH_3	—
Alkene	C=C		double bond
Alkyne	—C≡C—	H—C≡C—H	triple bond
Aromatic compound			phenyl group

Aliphatic Hydrocarbons

Aliphatic hydrocarbons have three subgroups.
Alkanes have only C—C bonds and no functional group.
Alkenes have a C—C double bond.
Alkynes have a C—C triple bond.

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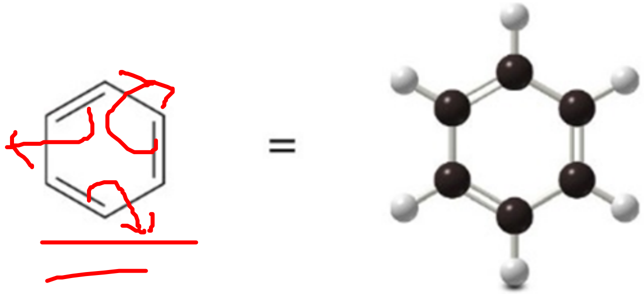
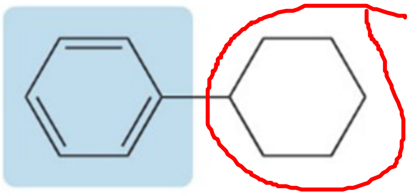
Aromatic Hydrocarbons

Aromatic hydrocarbons are so named because many of the earliest known aromatic compounds had strong, characteristic odors.
The simplest aromatic hydrocarbon is benzene.
The six-membered ring and three bonds of benzene comprise a single functional group, found in most aromatic compounds.



benzene
molecular formula C_6H_6



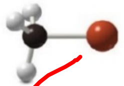
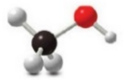
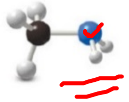
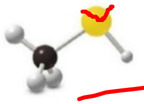
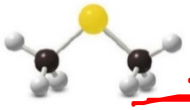
phenyl group
C_6H_5-
phenylcyclohexane

O, N, S etc

Functional Groups with Carbon- Heteroatom (C–Z) σ bonds

Several types of functional groups contain C—Z bonds.
The electronegative heteroatom Z creates a polar bond, making carbon electron deficient.

Functional Groups with C–Z σ bonds

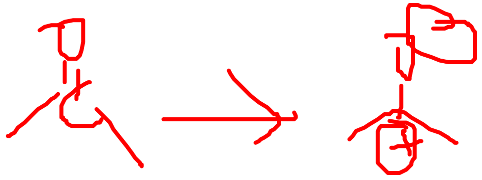
Type of compound	General structure	Example	3-D structure	Functional group
Alkyl halide	R–X: (X = F, Cl, Br, I)	CH_3–Br:		**–X** halo group
Alcohol	R–ÖH	CH_3–Ö–H		**–OH** hydroxy group
Ether	R–Ö–R	CH_3–Ö–CH_3		**–OR** alkoxy group
Amine	R–N̈H_2 or R_2N̈H or R_3N̈	CH_3–N̈H–H		**–NH_2** amino group
Thiol	R–S̈H	CH_3–S̈–H		**–SH** mercapto group
Sulfide	R–S̈–R	CH_3–S̈–CH_3		**–SR** alkylthio group

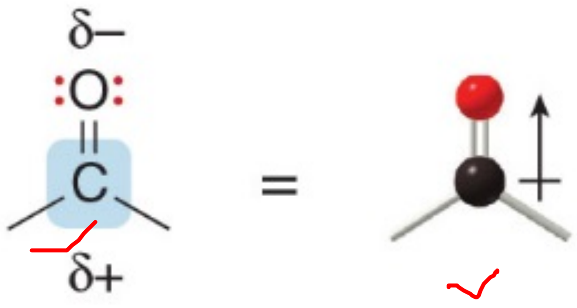
Functional Groups with C=O Group

This group is called a "carbonyl group".

The polar C—O bond makes the carbonyl carbon an electrophile, while the lone pairs on O allow it to react as a nucleophile and base.

The carbonyl group also contains a bond that is more easily broken than a C—O bond.





carbonyl group

Functional Groups with C=O Group-1

Type of compound	General structure	Example	Condensed structure	3-D structure	Functional group
Aldehyde			CH_3CHO		
Ketone			$(CH_3)_2CO$		carbonyl group
Carboxylic acid			CH_3CO_2H		carboxy group
Ester			$CH_3CO_2CH_3$		
Amide	H (or R) H (or R)		CH_3CONH_2		
Acid chloride			CH_3COCl		

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Importance of Functional Groups

A functional group determines all of the following properties of a molecule:

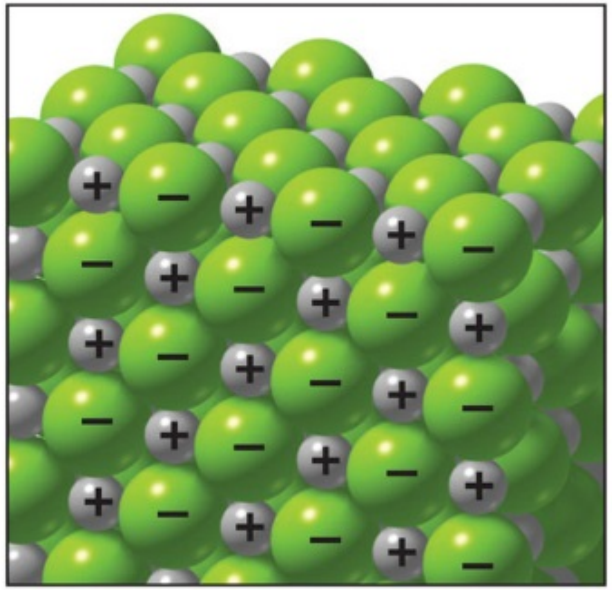
- bonding and shape
- type and strength of intermolecular forces
- physical properties
- nomenclature
- chemical reactivity

Intermolecular Forces

Intermolecular forces are interactions that exist between molecules.
Functional groups determine the type and strength of these interactions.
Ionic and covalent compounds have very different intermolecular interactions.

Ion-Ion Interactions

Ionic compounds contain oppositely charged particles held together by extremely strong electrostatic interactions. These ionic interactions are much stronger than the intermolecular forces present between covalent molecules.



strong electrostatic interaction between Na^+ and Cl^-

Intermolecular Forces in Covalent Molecules

Covalent compounds are composed of discrete molecules.
The nature of the forces between molecules depends on the functional group(s) present.
There are three different types of interactions, shown below in order of increasing strength:
van der Waals forces
dipole-dipole interactions
hydrogen bonding

Vander Wal Forces

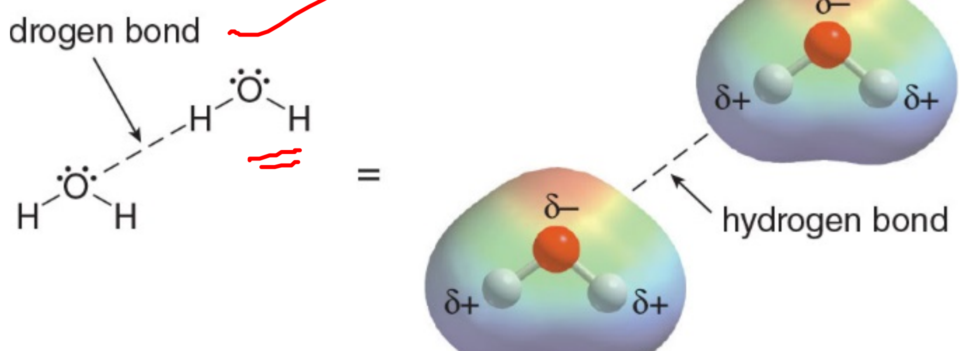
van der Waals forces are also known as London forces.
They are very weak interactions caused by momentary changes in electron density in a molecule.
They are the only attractive forces present in nonpolar compounds.

Dipole-Dipole Interactions

Dipole-dipole interactions are the attractive forces between the permanent dipoles of two polar molecules.
The dipoles in adjacent molecules (e.g., acetone below) align so that the partial positive and partial negative charges are in close proximity.
These attractive forces caused by permanent dipoles are much stronger than weak van der Waals forces.

Hydrogen Bonding

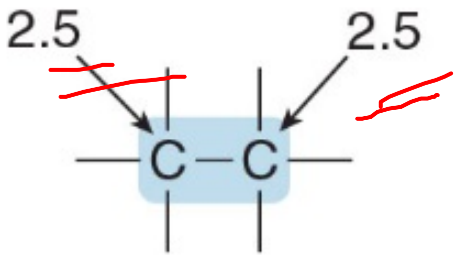
Hydrogen bonding typically occurs when a hydrogen atom bonded to O, N, or F, is electrostatically attracted to a lone pair of electrons on an O, N, or F atom in another molecule.
Hydrogen bonding is the strongest of the three types of intermolecular forces.



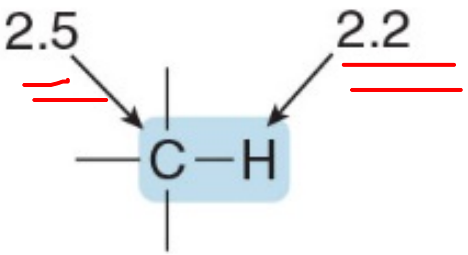
Bond Polarity

Electronegativity values are used to indicate whether the electrons in a bond are equally shared or unequally shared between two atoms.

When electrons are equally shared, the bond is nonpolar.



nonpolar bond



nonpolar bond

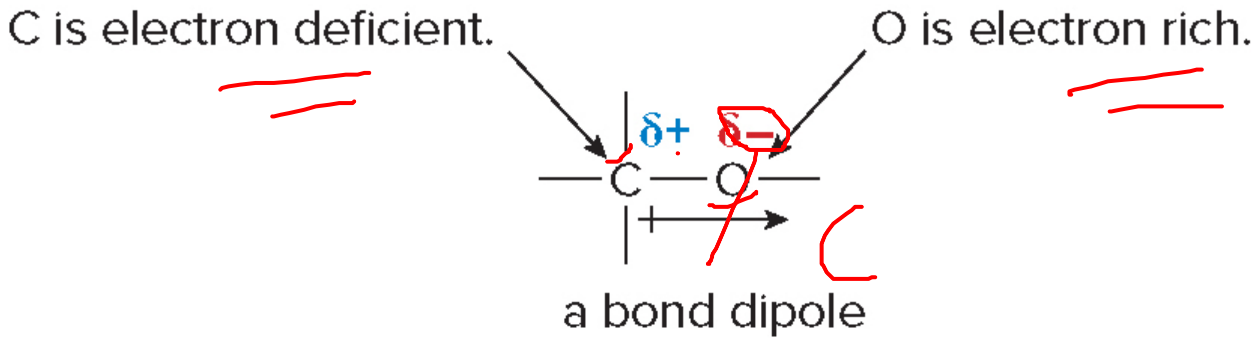
The small electronegativity difference between C and H is ignored.

Nonpolar Bonds

A carbon—carbon bond is nonpolar.
C—H bonds are considered to be nonpolar because the electronegativity difference between C and H is small.
Whenever two different atoms having similar electronegativities are bonded together, the bond is nonpolar.

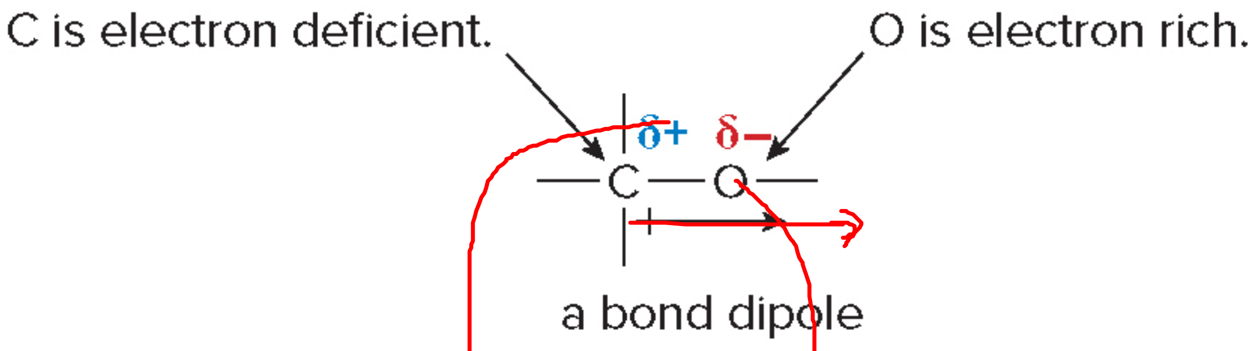
Polar Bonds

Bonding between atoms of different electronegativity values results in unequal sharing of electrons.
Example: In the C—O bond, the electrons are pulled away from C (2.5) toward O (3.4), the element of higher electronegativity. The bond is polar, or polar covalent. The bond is said to have dipole; that is, partial separation of charge.



A C—O bond is a polar bond.

Depicting Polarity



The δ+ means the indicated atom is electron deficient.
The δ− means the indicated atom is electron rich.
The direction of polarity in a bond is indicated by an arrow with the head of the arrow pointing towards the more electronegative element.
The tail of the arrow is drawn at the less electronegative element.