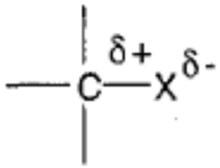
Organic chemistry background II

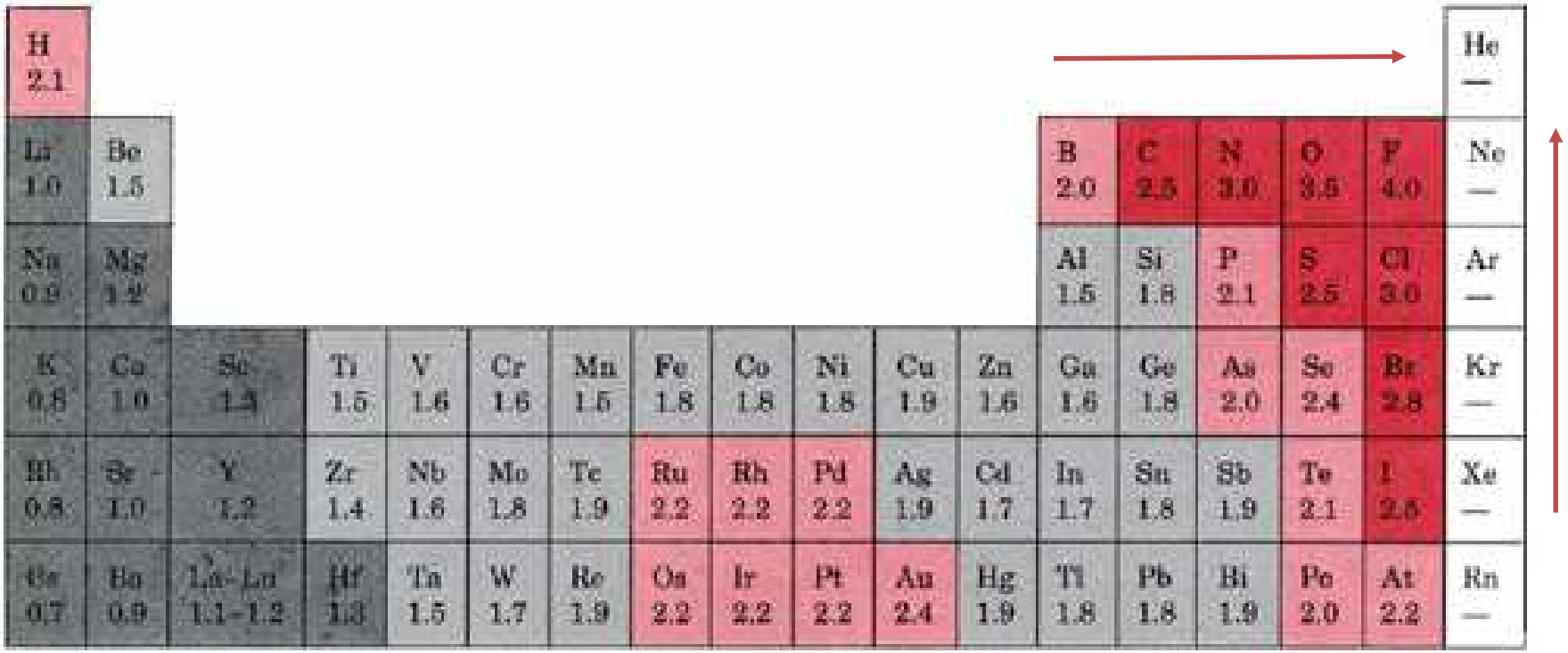
Electronegativity

- The “electron cloud” or averaged electron position located between the two nuclei is, in general, distorted toward the atom that has the higher attraction for the electrons (the atom that is more ***electronegative***)
  - ex: carbon-halogen bond



- Electronegativity increases with increasing kernel size within a row in the Periodic Table and decreases with increasing kernel size within a column

Electronegativity



ref: http://chemwiki.ucdavis.edu/Inorganic_Chemistry/Descriptive_Chemistry/Periodic_Trends_of_Elemental_Properties/Periodic_Trends

Oxidation state

- For convenience, assign the possession of the electron pair in a covalent bond to the more electronegative atom

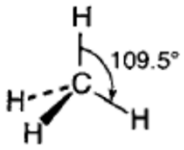
- Add 0 for each bond to an identical atom; -1 for each bond to a less electronegative atom or for each negative charge on the atom; +1 for each bond to a more electronegative atom or for each positive charge on the atom

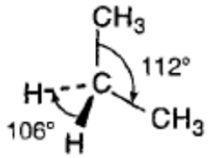
Oxidation state

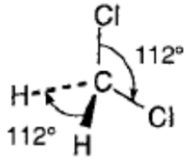
Q: Determine the oxidation state of each atom in acetate (CH_3COO^-).

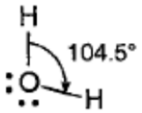
Spatial arrangement of atoms

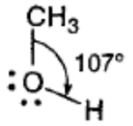
- Each pair of electrons, shared or unshared, wants to stay as far as possible from one another
  - For a carbon atom with four single bonds will form a tetrahedron
  - When carbon is bound to four identical atoms or groups (ex: CH_4), the bond angles should be 109.5°
  - The difference of the atoms or groups bound to a carbon leads to minor variations in the bond angles

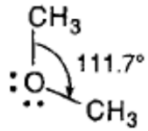

H
109.5°
C
H
H
H

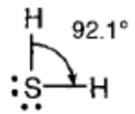

CH3
112°
H
C
CH3
106°
H

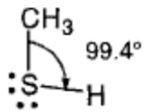

Cl
112°
H
C
Cl
112°
H

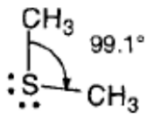

H
104.5°
O
H

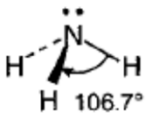

CH3
107°
O
H

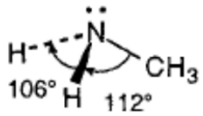

CH3
111.7°
O
CH3

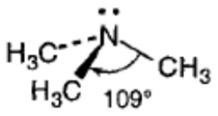

H
92.1°
S
H

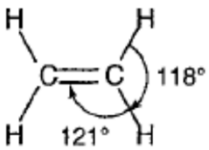

CH3
99.4°
S
H

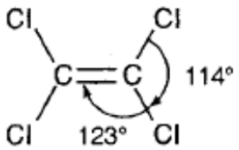

CH3
99.1°
S
CH3

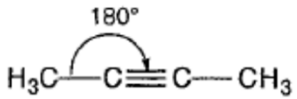

N
H
H
H
106.7°

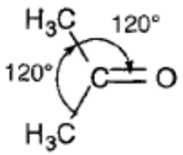

N
H
CH3
106°
H
112°

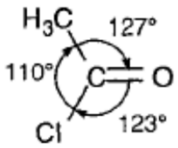

N
H3C
CH3
H3C
109°

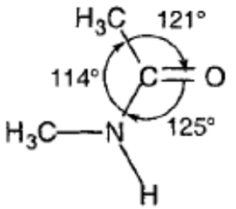

H
H
C
C
118°
H
121°
H


Cl
Cl
C
C
114°
Cl
123°
Cl


180°
H3C
C
C
CH3


H3C
120°
120°
C
O
H3C


H3C
127°
110°
C
O
Cl
123°


H3C
121°
114°
C
O
H3C
N
125°
H

Isomers

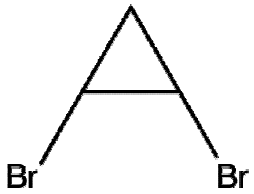
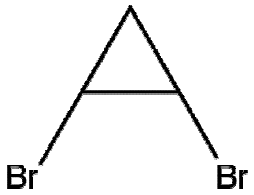
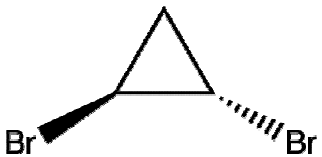
- **(Structural) Isomers**: the set of compounds whose molecular formula is identical, but the molecular structures are different

- **Stereoisomers**: the set of compounds whose molecular structure is identical, but the spatial arrangements are different

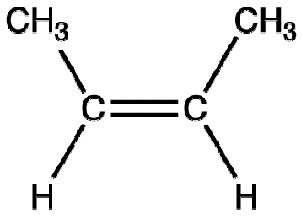
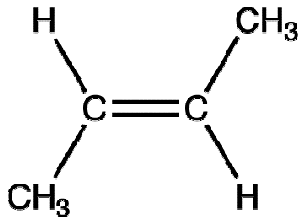
Isomers

Q: How many (structural) isomers are there for monochlorinated butane (C_4H_9Cl)? Draw the chemical structures of all isomers.

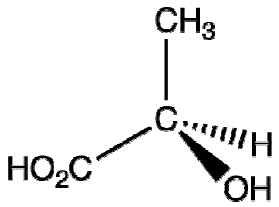
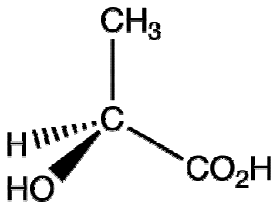
Stereoisomers

	cis–1,2–dibromo cyclopropane **(1)**	*trans*–1,2–dibromo cyclopropane **(2)**
molecular formula	$C_3H_4Br_2$	$C_3H_4Br_2$
structural formula		
configuration		

Stereoisomers

	cis–2–butene **(1)**	*trans*–2–butene **(2)**
molecular formula	C_4H_8	C_4H_8
structural formula	$CH_3CH{=}CHCH_3$	$CH_3CH{=}CHCH_3$
configuration		

Stereoisomers

	(*R*)–lactic acid (**1**)	(*S*)–lactic acid (**2**)
molecular formula	$C_3H_6O_3$	$C_3H_6O_3$
structural formula	CH_3CHCO_2H | OH	CH_3CHCO_2H | OH
configuration		

Stereoisomers

Q: Are there any pair of stereoisomers among structural isomers of monochlorinated butane?