

Chapter 1. Electronic Structure and Covalent Bonding

Learning objectives:

1. Write the ground-state electron configuration.
2. Draw Lewis structure.
3. Use electronegativity to predict polarized and non-polarized bond.
4. Predict the hybridization, bond angles, and geometry of an atom or molecule.
5. Recognize polar and non-polar molecules

Sections to be covered:

- 1.1 The structure of an atom
- 1.2 How the electrons in an atom are distributed
- 1.3 Ionic and covalent bonds
- 1.4 How the structure of a compound is represented*
- 1.5 Atomic orbitals
- 1.6 How atoms form covalent bonds*
- 1.7 How single bonds are formed in organic compounds
- 1.8 How a double bond is formed: the bonds in ethene
- 1.9 How a triple bond is formed: the bonds in ethyne
- 1.10 Bonding in the methyl cation, the methyl radical, and the methyl anion
- 1.11 The bonds in water
- 1.12 The bonds in ammonia and in the ammonium ion
- 1.13 The bond in hydrogen halide
- 1.14 Summary: hybridization, bond lengths, bond strengths, and bond angles

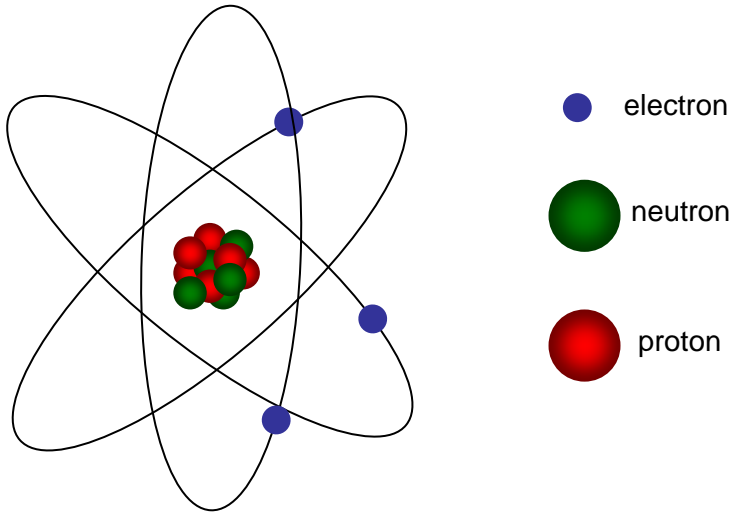
* Sections that will be focused

Sections that will be skipped

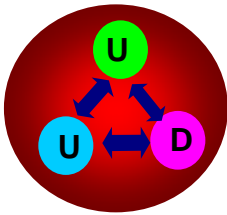
Recommended additional problems

31, 33, 34, 37, 42, 45, 46, 48, 52,

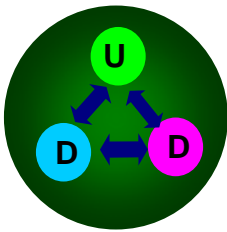
1.1 The structure of an atom



Proton consists of two up quarks and one down quark.



Neutron consists of two down quarks and one up quark.



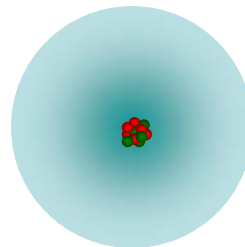
Know the following glossaries:

Atomic number:

Atomic weight (atomic mass)

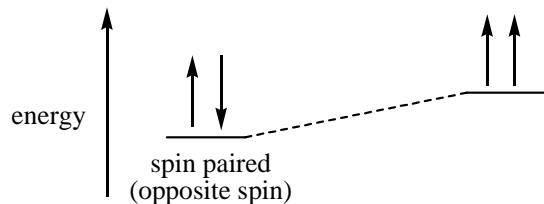
Isotope:

1.2 How the electrons in an atom are distributed



A. Electron Configuration of Atoms

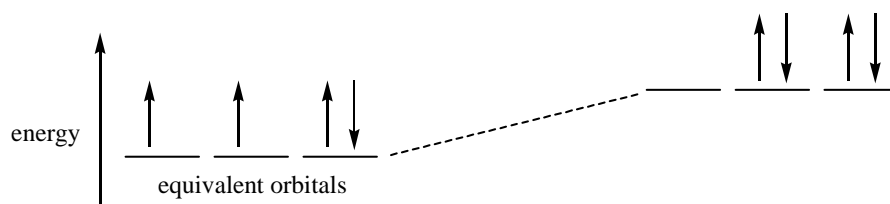
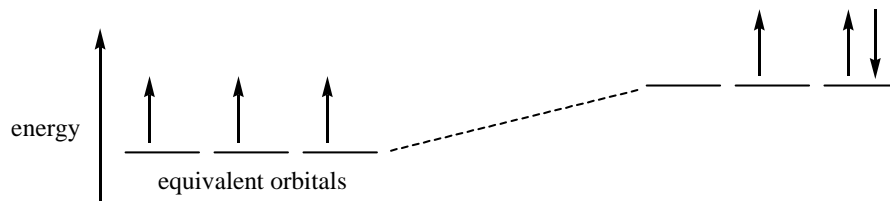
(i) Each atomic orbital can hold up to two electrons with their spin paired (opposite spin).



(ii) Fill electrons into atomic orbitals in order of increasing energy from lowest to highest.

Know the energy level of basic atomic orbitals.

(iii) For orbitals with equivalent energy, fill in one electron to each equivalent orbital before completely filling any one of these equivalent orbitals.



Examples:

H:

He:

Li:

C:

N:

O:

Na:

P:

Know the difference between valence and core electrons.



1.3 Ionic and covalent bonds

A. Formation of Ions (Octet rule, Anion and Cation)

Na

Mg

F

B. Formation of Chemical Bond

Ionic bond (charge attraction)



Covalent bond (sharing electrons)



C. Electronegativity and Chemical Bonds

(i) Tendency of electronegativity on periodic table

(ii) Important electronegativity

H:

F:

Li:

C:

N:

O:

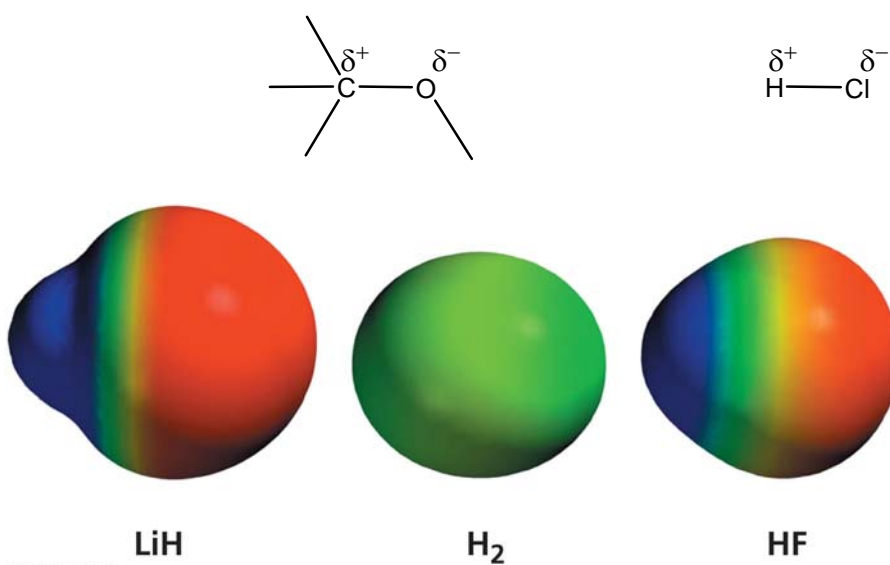
(iii) Electronegativity and chemical bonds

Ionic bond

Polar bond

Covalent bond

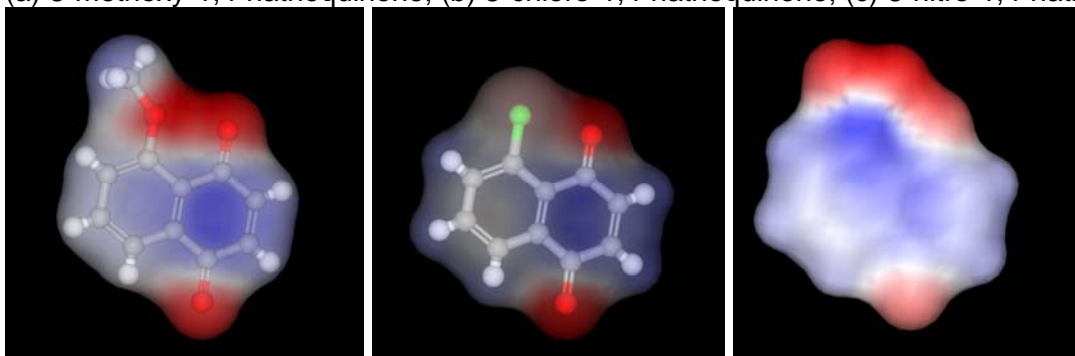
D. Electrostatic potential maps



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Electron-density distribution (left to right):

(a) 8-methoxy-1,4-nathoquinone; (b) 8-chloro-1,4-nathoquinone; (c) 8-nitro-1,4-nathoquinone.



1.4 How the structure of a compound is represented

A. Lewis Structures of Molecules and Ions

(i) Determine the number of valence electrons

(ii) Know the number of legible (optimal) bonds and lone pair electrons for the commonly seen atoms:

H C N O F (Cl, Br, I)

(iii) Determine the arrangement of atoms.

Identify the Center Atom(s)

(iv) Show the chemical bond as single line and non-bonding electrons as a pair of Lewis dots.

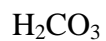
(v) Use multiple bonds when necessary

double and triple bond

(vi) Pay attention to the octet rule

(vii) Avoid but not exclude O-O, O-X and three membered ring

Examples:



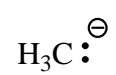
B. Formal Charge

(i) Know the number of valence electrons for the commonly seen atoms.

(ii) Know the number of legible (optimal) bonds and the corresponding charge for the commonly seen atoms.

(iii) Arrange atoms according to the guidelines of section 1.4.A.

Examples:



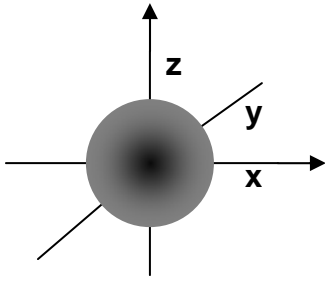
C. Kekulé Structures

Use line to represent chemical bond.

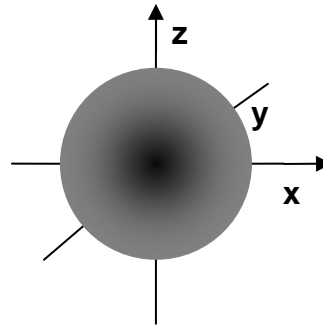
Lone-pair electron can be omitted.

D. Condensed Structures

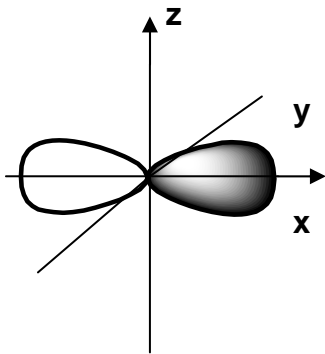
1.5 Atomic orbitals



1s orbital



2s orbital



2p_x orbital

P orbitals have different phase.

1.6 How atoms form covalent bonds

Overlapping between:

A. 1s and 1s

B. 1s and 2p (head on vs. side way)

C. 2p and 2p (head on and side way)

1.7 How single bonds are formed in organic compounds

Know the concept of hybridization.

A. Hybridization provides same number of hybridized orbitals.

Example: 1s hybridizes with one 2p orbital

B. Hybridization determines the geometry.

Know the total number of σ bond(s) and lone-pair electron(s) for the center atom(s)

Examples:



(ii) Difference of σ bond and π bond

(iii) Lone-pair electrons will not be considered as part of the shape of molecule.

(iv) The total number of σ bond(s) and lone-pair electron(s) for the center atom(s) dictate the arrangement of atoms surrounding the center atom(s) thus shape of molecules around the center atom(s).

Total Number	Description of Shape	Predicted Bond Angles	Possible Variation	Hybridization of Center Atom(s)
2	Linear	180°		SP
3	Trigonal Planar	120°	Linear-like (two pairs of lone-pair electrons) Bent (planar, one pair of lone-pair electrons)	SP ²
4	Tetrahedral	109.5°	Bent (planar, two pairs of lone-pair electrons) Pyramidal (one pair of lone-pair electrons)	SP ³

C. Examples: methane (CH₄) and ethane (CH₃CH₃)

SP hybridization: two sp hybridized orbitals and two 2p (2p_y and 2p_z) orbitals

SP² hybridization: three sp² hybridized orbitals and one 2p (2p_z) orbital

SP³ hybridization: four sp³ hybridized orbitals and no 2p orbital left

1.8 How a double bond is formed: the bonds in ethane

1.9 How a triple bond is formed: the bonds in ethyne

1.10 Bonding in the methyl cation, the methyl radical, and the methyl anion

1.11 The bonds in water

1.12 The bonds in ammonia and in the ammonium ion

1.13 The bond in hydrogen halide

1.14 Summary: hybridization, bond lengths, bond strengths, and bond angles

A. Polarity of molecules

Examples:

(i) CO_2

(ii) CH_3OH

(iii) CH_3NH_2

(iv) CF_4

(v) CH_3Cl

(vi) CH_3COCH_3