

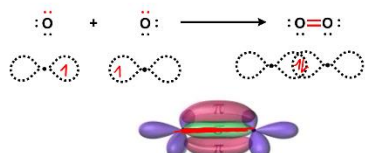
Major Concepts Covered (these questions cover all lectures from 1 to 21 and serve as a practice for the midterm)

Theories of Covalent Bonding (Hybridization/VSEPR)

Valence Bond Theory:

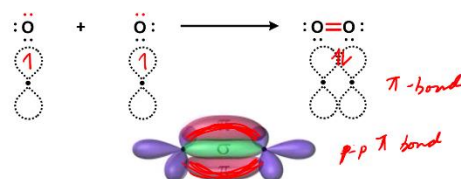
Formation of single and double bonds

A covalent bond forms when orbitals of two atoms overlap and a pair of electrons occupy the overlap region



σ -bond – formed from overlap of two orbitals. Is cylindrically symmetrical around bond axis

- The two electrons move over to the new **σ -bonding** orbital
- The two electrons in the bonding orbital have opposite spin (Pauli's exclusion principle still followed)



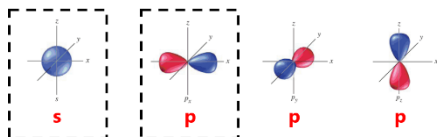
π -bond – formed from overlap of two orbitals. Is not symmetrical around bond axis. Side to side overlap

- The two electrons move over to the new **π -bonding** orbital
- The two electrons in the bonding orbital have opposite spin (Pauli's exclusion principle still followed)

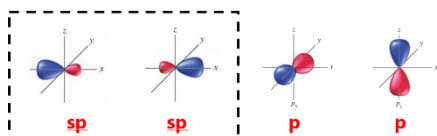
Hybridization

sp

Atomic Be
Valence
Orbitals:

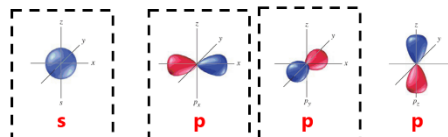


Be atoms in BeCl₂
Valence
Orbitals:

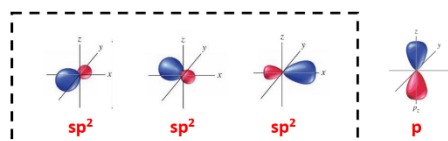


sp²

Atomic B
Valence
Orbitals:

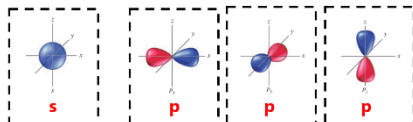


B atoms in BF₃
Valence
Orbitals:

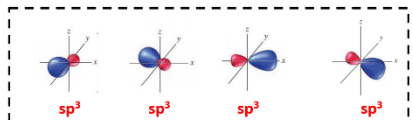


sp³

Atomic B
Valence
Orbitals:

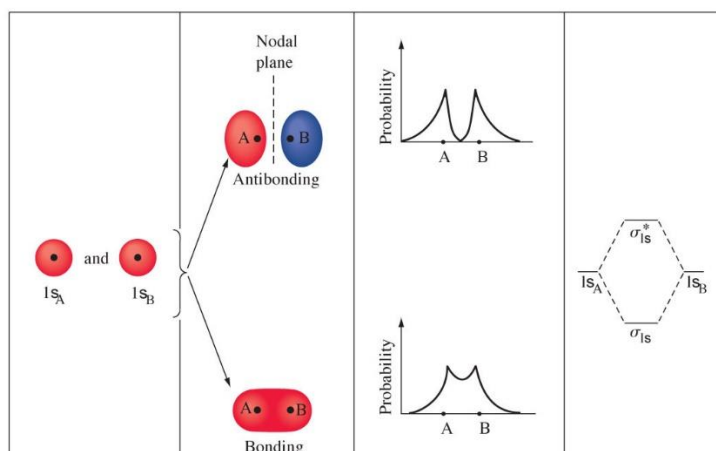


C atoms in CH₄
Valence
Orbitals:



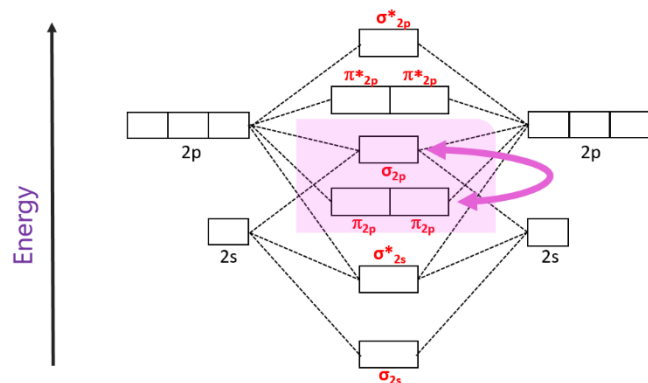
Molecular Orbital Theory

Period 1: Drawing Molecular Orbital Diagram

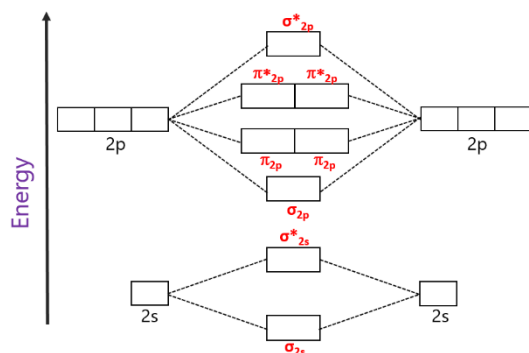


Period 2:

MO Diagram for Li_2 to N_2



MO Diagram for O_2 and F_2



Be able to determine bond order, compare bond length, magnetism, and write molecular configuration

Tutorial Questions (these questions cover all lectures from 1 to 21 and serve as a practice for the midterm)

The subsequent ionization energies (in kJ/mol) for an imaginary element (X) are given below.

	IE ₁	IE ₂	IE ₃	IE ₄	IE ₅	IE ₆	IE ₇	IE ₈
X	1215	2214	3123	13215	15612	18145	23412	28361

a) Which main group would you place this element in? Briefly explain your reasoning. 3 points

Biggest jump from IE₃ to IE₄

Group 13

b) Calculate the longest wavelength (in nm) of a photon that can remove an electron from the ground state atom X (from part a)? Show complete calculations. 3 significant figures 7 points

LONGEST WAVELENGTH = SMALLEST ENERGY
IE₁ = 1215 kJ/mol → Easiest to remove electron

$$\Delta E = \frac{1215 \text{ kJ}}{\text{mol}} = 1215 \times 10^3 \frac{\text{J}}{\text{mol}} \quad \leftarrow 1 \text{ mol} = 6.023 \times 10^{23} \text{ photons/mole}$$

$$\Delta E_{\text{photon}} = \frac{1215 \times 10^3 \text{ J}}{\text{mol}} \times \frac{1}{6.023 \times 10^{23} \text{ photon}} \text{ mol}$$

$$= \frac{1215 \times 10^{-20} \text{ J}}{6.023}$$

$$\Delta E = \frac{hc}{\lambda}$$

$$\frac{1215 \times 10^{-20} \text{ J}}{6.023} = \frac{(6.626 \times 10^{-34} \text{ J}\cdot\text{s}) (2.998 \times 10^8 \text{ m/s})}{\lambda}$$

$$\lambda = \frac{6.626 \times 10^{-34} \times 2.998 \times 10^8 \times 6.023}{1215 \times 10^{-20}} \text{ m}$$

$$= 0.0985 \times 10^{-6} \text{ m}$$

$$= 98.5 \text{ nm}$$

2)

2)

- a) The work function of the metal is 1.42×10^{-18} J. Among the given wavelengths (i, ii, iii, or iv), which is the *longest wavelength* that will cause an electron to be ejected from the surface? Show calculations to explain your answer. **6**

(i) 50 nm

(ii) 100 nm

(iii) 150 nm

(iv) 200 nm

- a) The work function of the metal is 1.42×10^{-18} J. Among the given wavelengths (i, ii, iii, or iv), which is the *longest wavelength* that will cause an electron to be ejected from the surface? Show calculations to explain your answer. **6 points**

(i) 50 nm

(ii) 100 nm

(iii) 150 nm

(iv) 200 nm

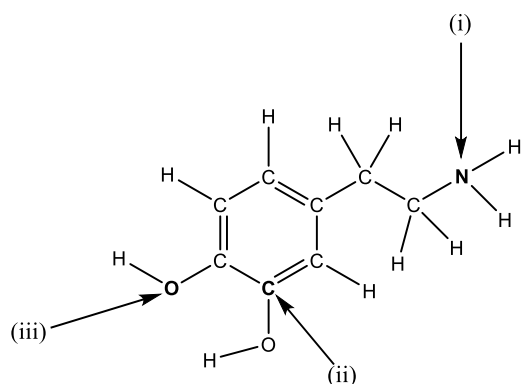
$$\phi = 1.42 \times 10^{-18} \text{ J} \quad \lambda_{\text{threshold}} = \frac{hc}{\phi} \approx 140 \text{ nm} \quad (\text{accept value between } 139 - 141 \text{ nm})$$

Wavelength must be below threshold to cause an electron to be ejected (frequency and wavelength are inversely related)

- b) Without doing any calculations, predict the change (increase, decrease, or no change) for the following, if the wavelength of the photon is shorter than the longest wavelength calculated in Part A.

- i. Work function of the metal: **NO CHANGE**
- ii. Velocity of the electron: **INCREASE**
- iii. Number of electrons ejected: **NO CHANGE**
- iv. Kinetic energy of the electron: **INCREASE**

3)



For the indicated atoms (denoted with an arrow), (i) to (iii), answer the following questions. Lone pairs are **not** indicated in the structure. Consider the structure as given (no need to consider resonance structures). All atoms have formal charge of 0. (Use valence bond theory and hybridization to describe the bonding.)

a) For (i)

1. Describe the orbitals involved in all bonds formed by N (i). Designate sigma and pi bonds

2sp³-s sigma bonds. 1 sp³-sp³ sigma bond

2. What is the electron **and** molecular geometry at N?

Electron geom: Tetrahedral; Molecule geom: Trigonal Pyramidal.

b) For (ii)

1. What is the molecular geometry at C (ii). Trigonal Planar

2. Circle the one value that best describes the O-C-C bond angle.

>90° to <109.5°

109.5°

120°

>120° to <180

c) For (iii)

1. What is the electron **and** molecular geometry at O (iii).

Electron geom: Tetrahedral; Molecule geom: Bent

2. Circle the one value that best describes the H-O-C bond angle.

>90° to <109.5°

109.5°

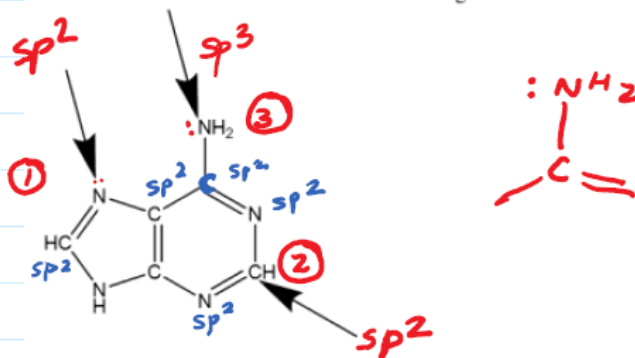
>109.5° to <120°

120°

>120° to <180

- 4) Consider the structure shown below.
In this structure all atoms have a formal charge of zero.

Consider the structure shown below.
In this structure all atoms have a formal charge of zero.



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- a. Identify the hybridization for the atoms indicated by the arrow

ACCOUNT FOR LONE PAIRS

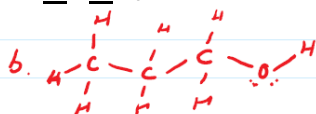
- b. Describe the orbitals involved in bonding for each atom indicated by an arrow.
Distinguish sigma and pi bonds for each.

① 2 $sp^2 - sp^2$ σ bonds (C-N)
1 p-p π bond (C-N)

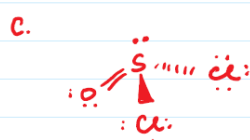
② 2 $sp^2 - sp^2$ σ bond (C-N)
1 p-p π bond (C-N)
1 $sp^2 - s$ σ bond (C-H)

③ 2 $sp^3 - s$ σ bond (N-H)
1 $sp^3 - sp^2$ σ bond (N-C)

5) Draw the Lewis structures, and predict the hybridization of the underlined atom(s). What is the molecular geometry around the underlined atom?

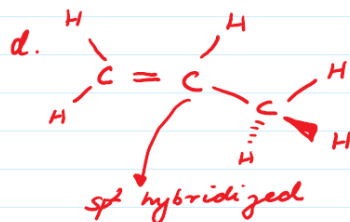


O: sp^3 hybridized
MOLECULAR GEOMETRY: BENT



S: sp^3 hybridized

MOLECULAR GEOM.: TRIGONAL PYRAMIDAL



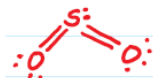
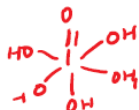
sp^2 hybridized

MOLECULAR GEOM.: TRIGONAL PLANAR

6. Based on what you have learned in Chem110, arrange the following in the increasing order of

1. Bond angle (for the most stable Lewis Structure)

(None of the molecules contain any O-O bonds)



$1 < 2 < 3$

H₅IO₆ is 90 degree octahedral

PH₃ is less than 109.5 (trig pyramidal)

SO₂ is less than 120 degree but greater than 109.5 (trigonal planar bent)

2. Ionic radius



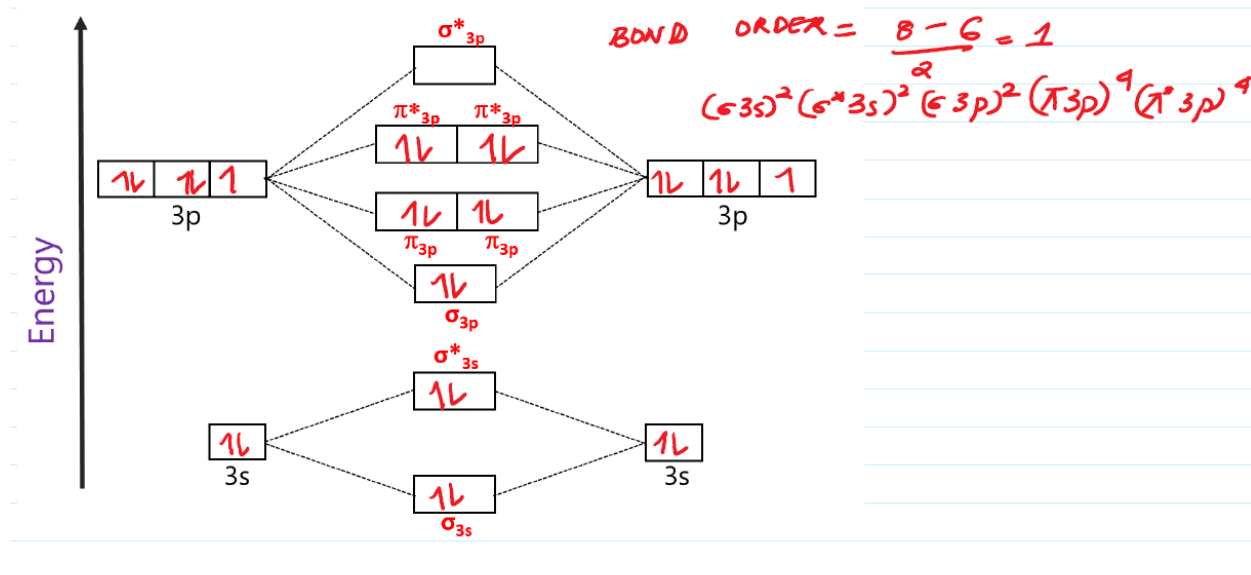
Briefly explain your reasoning for each.

On going down the group size increases so Sr > Ca and Sr²⁺ > Ca²⁺; (For similar reasons, I⁻ > Br⁻)

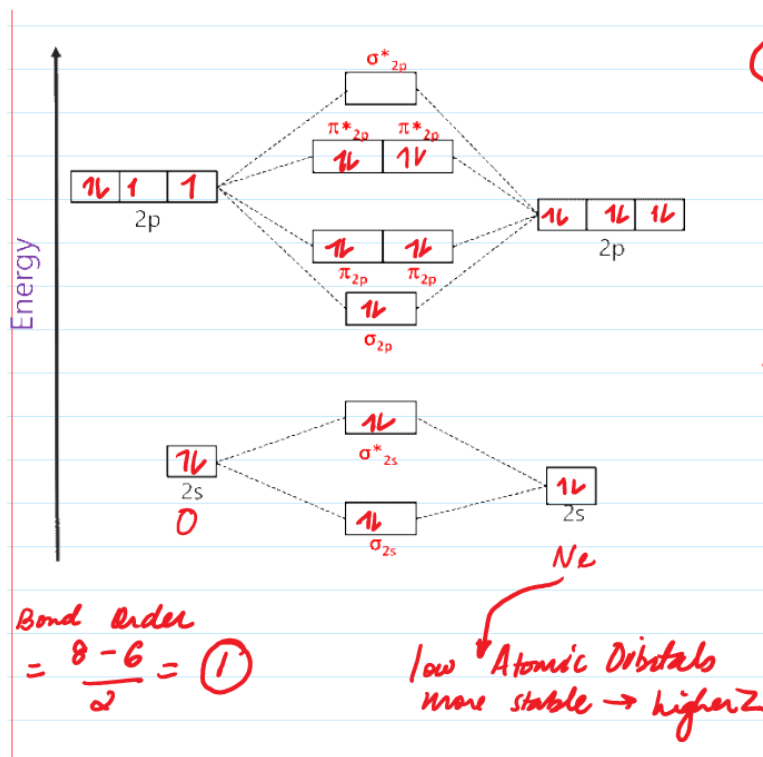
Sr²⁺ and Br⁻ are isoelectronic. Anions are larger than cations for isoelectronic species due to higher repulsions and lower effective nuclear charge. So Sr²⁺ < Br⁻ and hence is smaller than I⁻



7. Draw the molecular orbital diagram for Cl_2 . Assume 3s and 3p orbitals show similar LCAO as 2s and 2p orbitals (Label increasing energy using an arrow next to the diagram. Label each atomic and each molecular orbital)
- Calculate the bond order and give the molecular orbital configuration for the valence electrons.



8. a. Draw the complete MO diagram for the molecule NeO. Make sure to label atomic and molecular orbitals. Label the energy axis. What is the bond order?



- b. Arrange the following in the increasing order of their bond length

NeO, NeO⁻, NeO⁺

Explain your answer – based on MO theory.

⑥ Bond order
 NeO = 1

$$\text{NeO}^- = \frac{8 - 7}{2} = 0.5$$

$$\text{NeO}^+ = \frac{8 - 5}{2} = 1.5$$

Bond Length

$$\text{NeO}^- > \text{NeO} > \text{NeO}^+$$

(opposite trend of bond order)