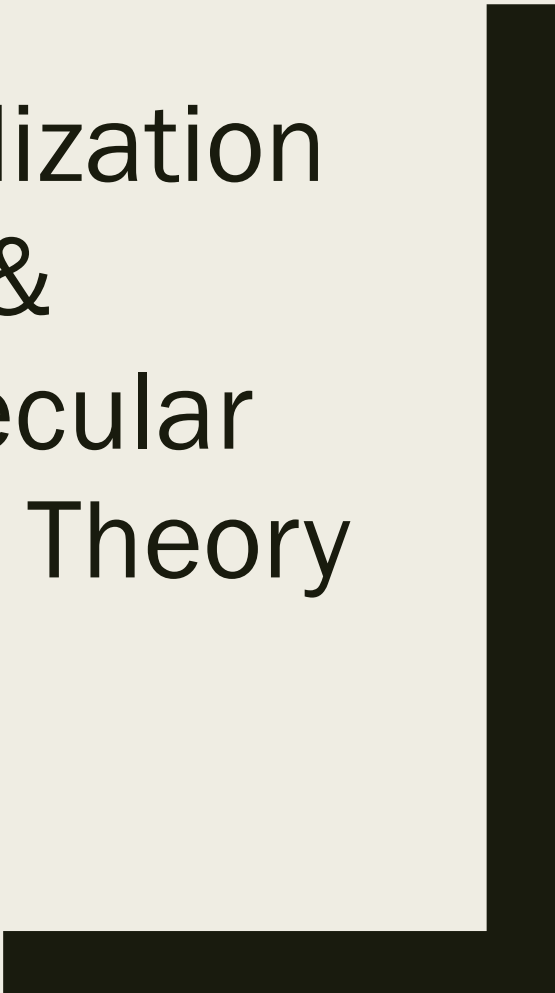


CHEM 101 DL

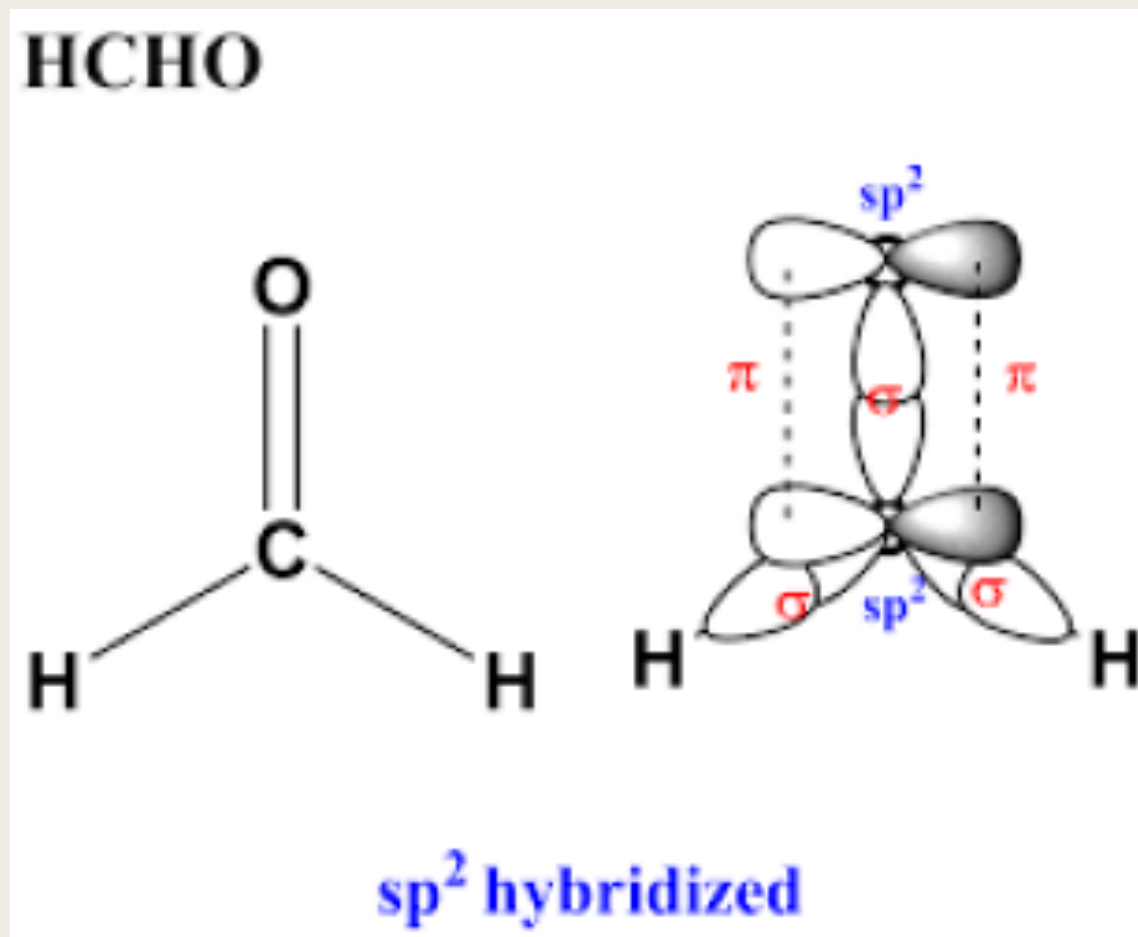
Chapter 14: Covalent Bonding

Feb 28th & Mar 2nd, 2023

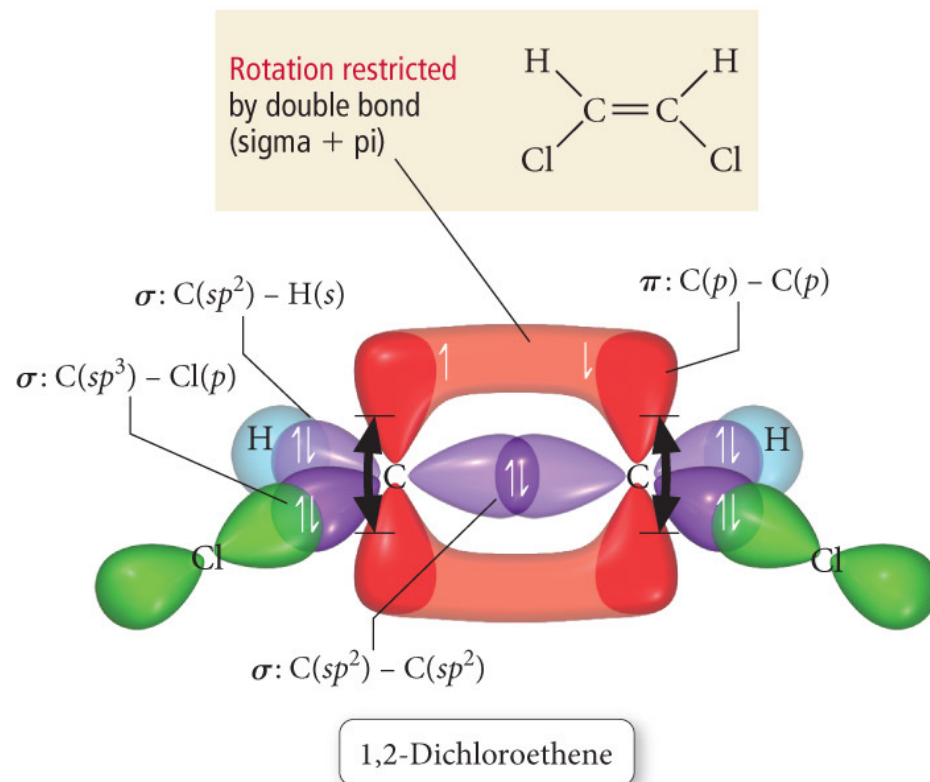
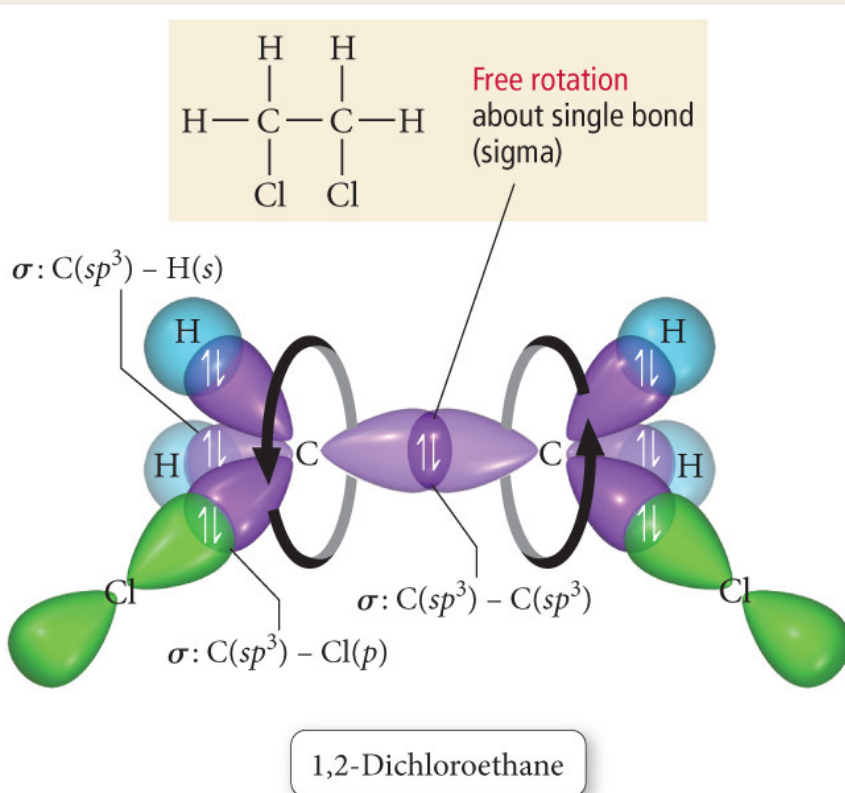
Hybridization & Molecular Orbital Theory



sp^2 hybridization – H_2CO



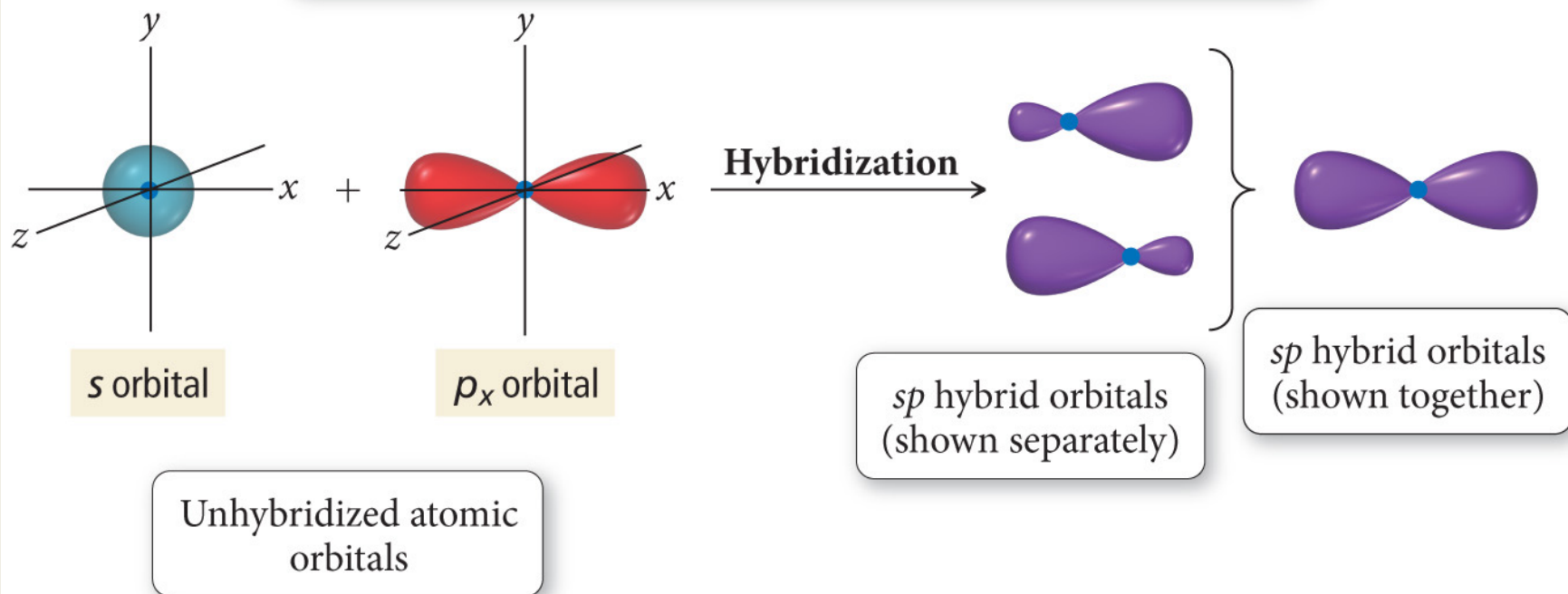
σ & π Bond Rotation



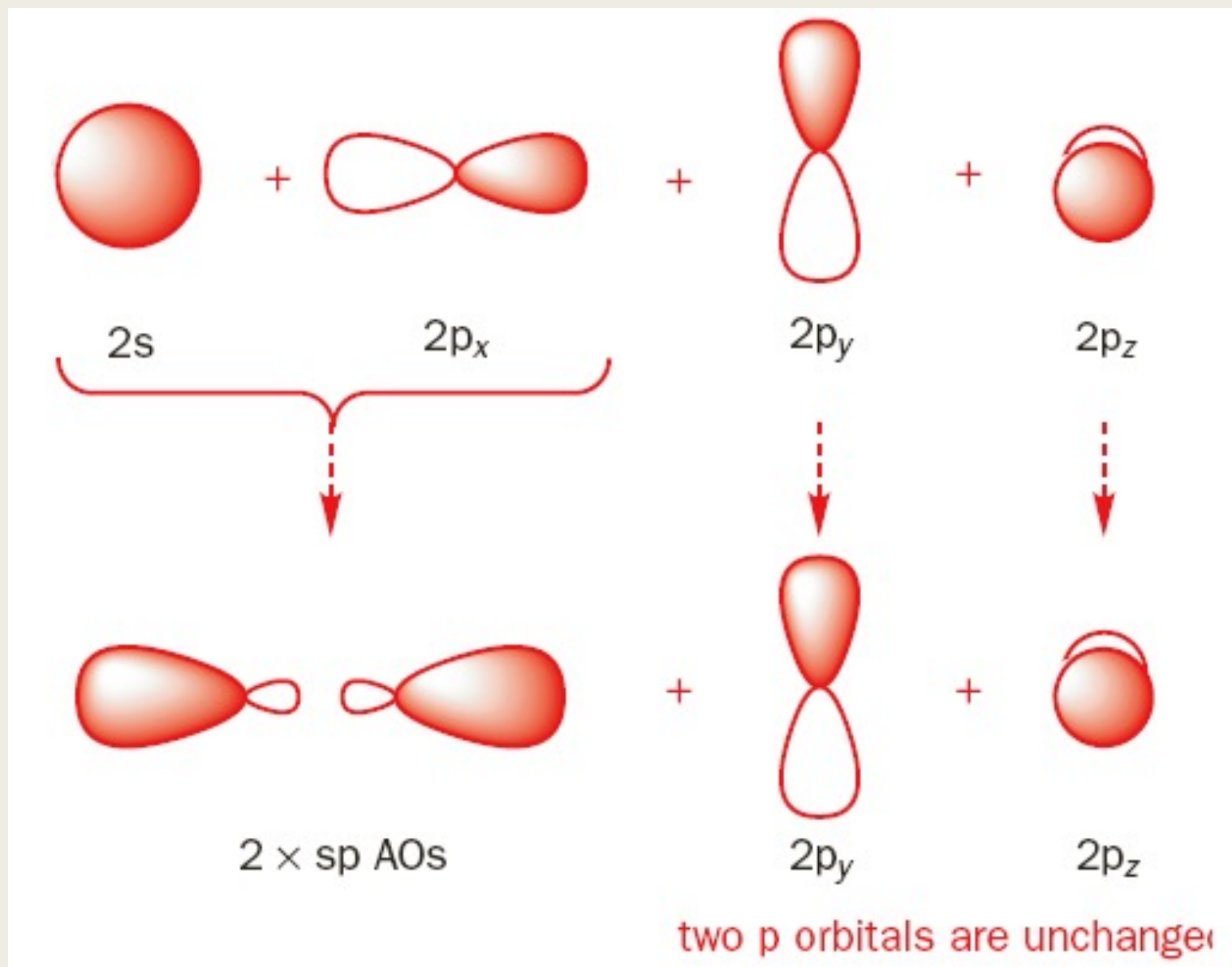
Formation of sp hybrid orbitals

Formation of sp Hybrid Orbitals

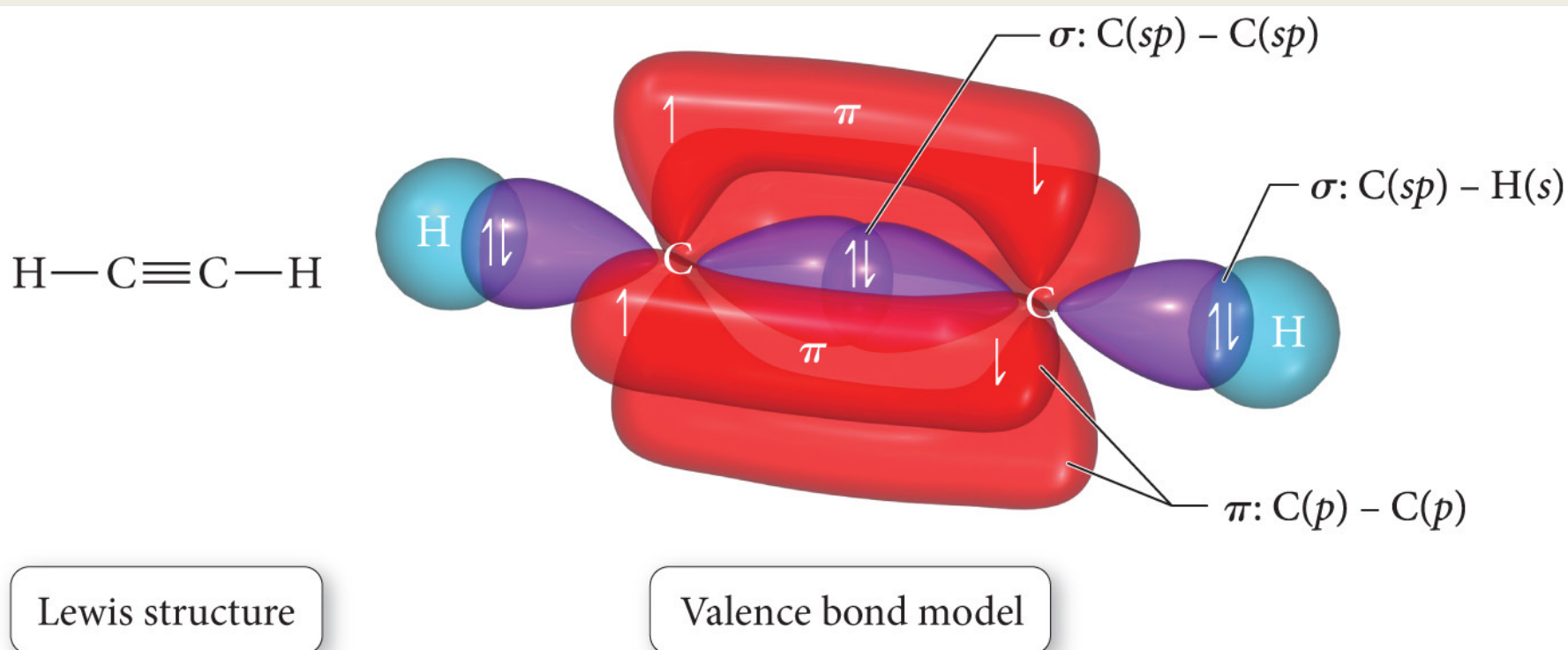
One s orbital and one p orbital combine to form two sp orbitals.



sp Hybridization

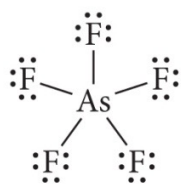


Formation of sp Hybrid Orbital in Ethyne

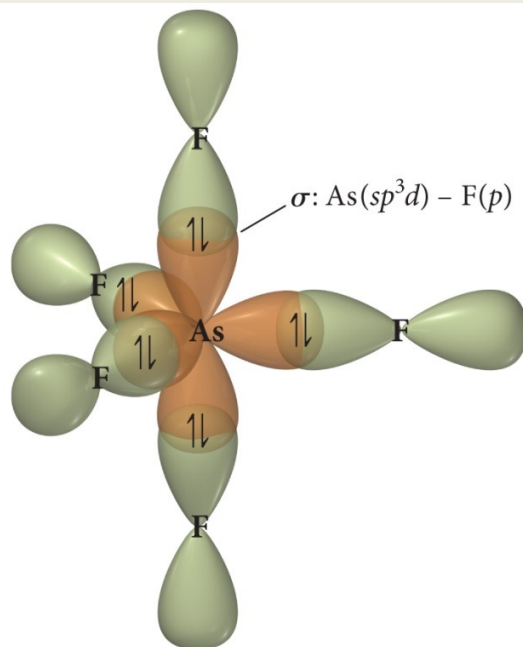


Triple bonds: 1 σ bond & 2 π bonds

sp^3d Hybridized Orbital

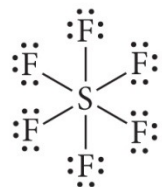


Lewis structure

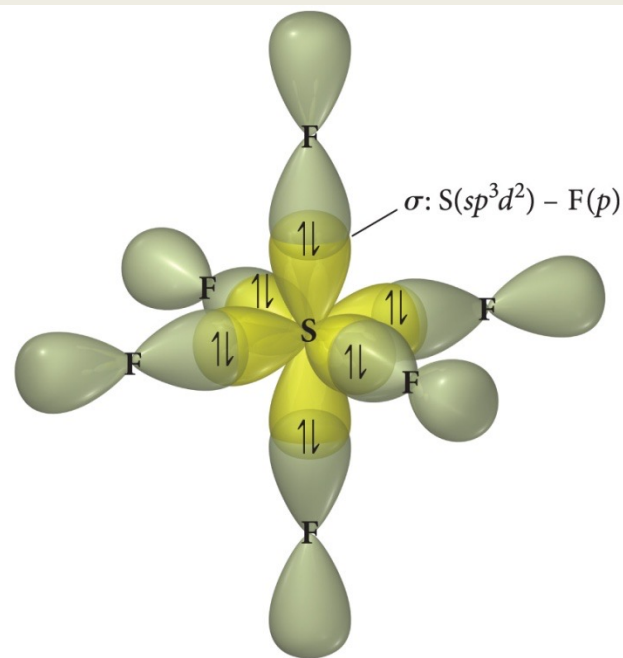


Valence bond model

sp^3d^2


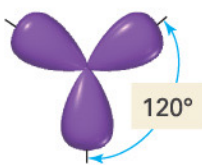
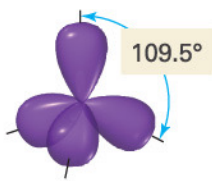
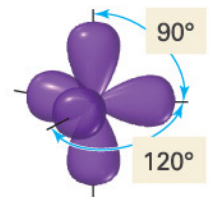
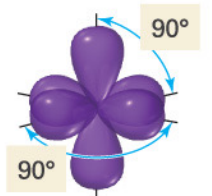


Lewis structure



Valence bond model

TABLE 7.1 Hybridization Scheme from Electron Geometry

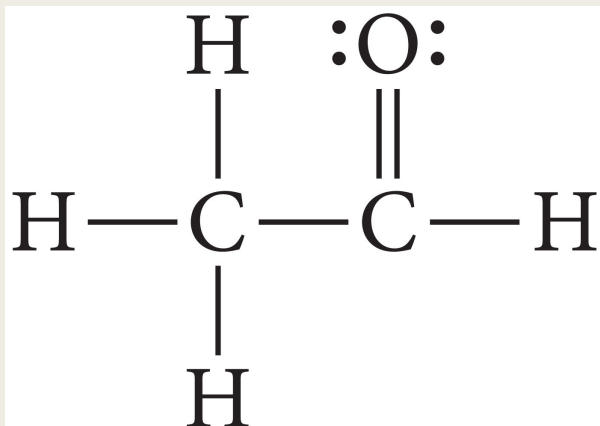
Number of Electron Groups	Electron Geometry (from VSEPR Theory)	Hybridization Scheme	Orbital Shapes and Relative Orientation
2	Linear	sp	
3	Trigonal planar	sp^2	
4	Tetrahedral	sp^3	
5	Trigonal bipyramidal	sp^3d	
6	Octahedral	sp^3d^2	

PRACTICE!

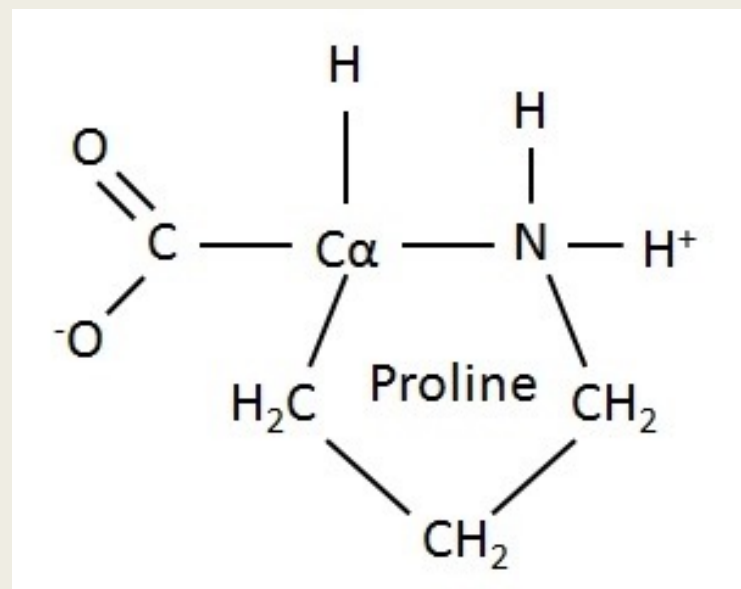
1. What type(s) of hybrid orbitals are present in CH_4 ?
2. What are the bond angles in methane?
3. What type of electron pair geometry is associated with sp hybrid orbitals?
4. What type of electron pair geometry is associated with sp^2 hybrid orbitals?
5. What is the hybridization of chlorine in the chlorate ion (ClO_3^-)?

PRACTICE!

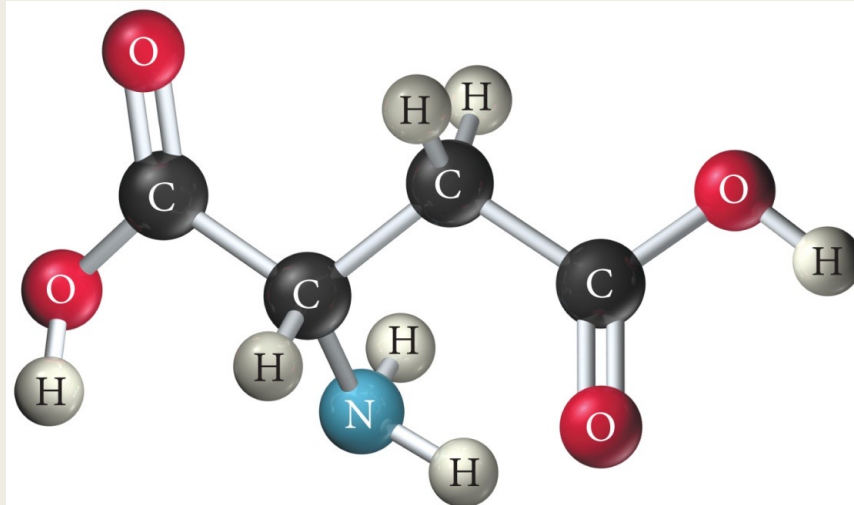
1. What is the hybridization of each of the carbon atoms?
2. How many sigma bonds does this molecule have?



How many central atoms in proline are sp^3 , sp^2 , and sp hybridized?



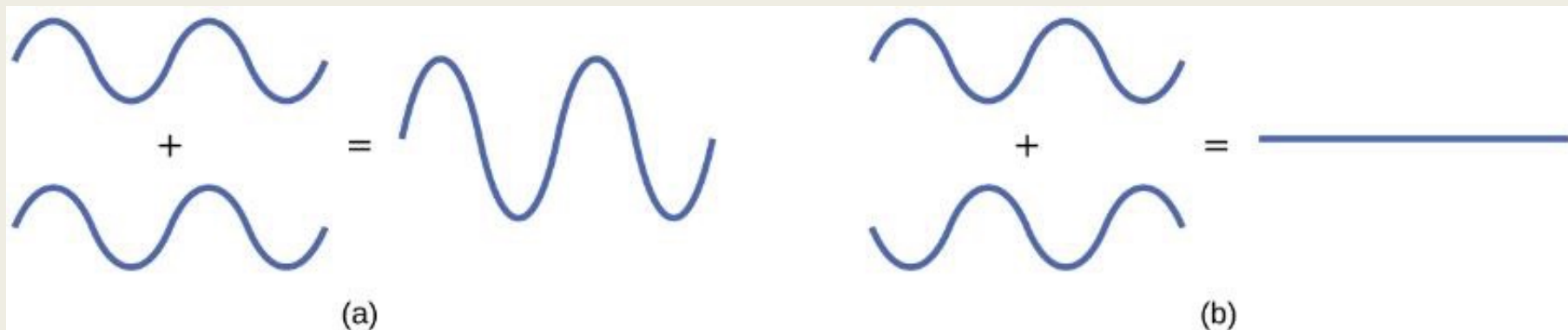
1. What is the hybridization of each of the central atoms?
2. How many π electrons are found in the amino acid aspartic acid?



Molecular Orbital Theory!

- Describe how approximate molecular orbitals in the MO approach are formed from linear combinations of atomic orbitals
- For diatomic molecules, be able to describe and sketch the sigma and pi bonding and anti-bonding orbitals that result from combinations of the s and p orbitals on the two atoms
- Use molecular orbital energy level diagrams to show how the electrons in a homonuclear diatomic molecule occupy the various molecular orbitals, and from this diagram determine the bond order, MO electron configuration, and the number of unpaired electron spins (hence paramagnetic vs diamagnetic)
- For a series of diatomic molecules, use bond orders to determine their relative stabilities, bond lengths, and bond energies
- Extend the use of molecular energy level diagrams described above to heteronuclear diatomic molecules and diatomic molecular ions

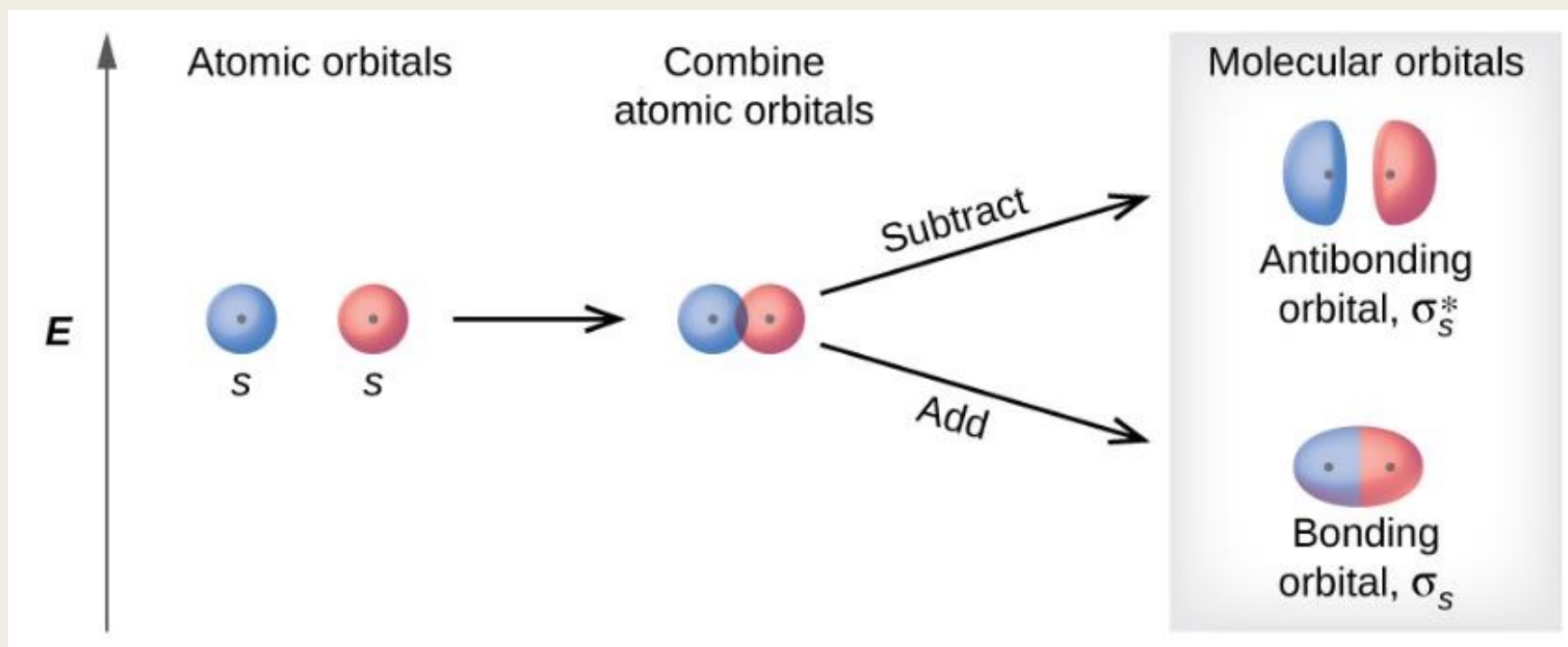
Interference with Waves



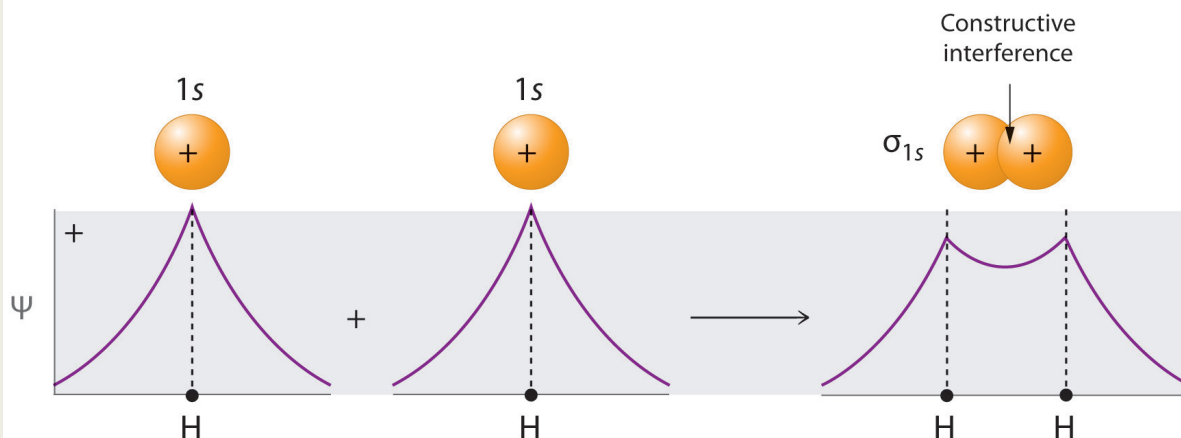
Constructive Interference

Destructive Interference

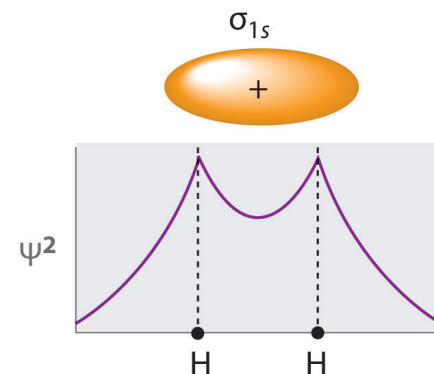
Interference with s-Orbitals



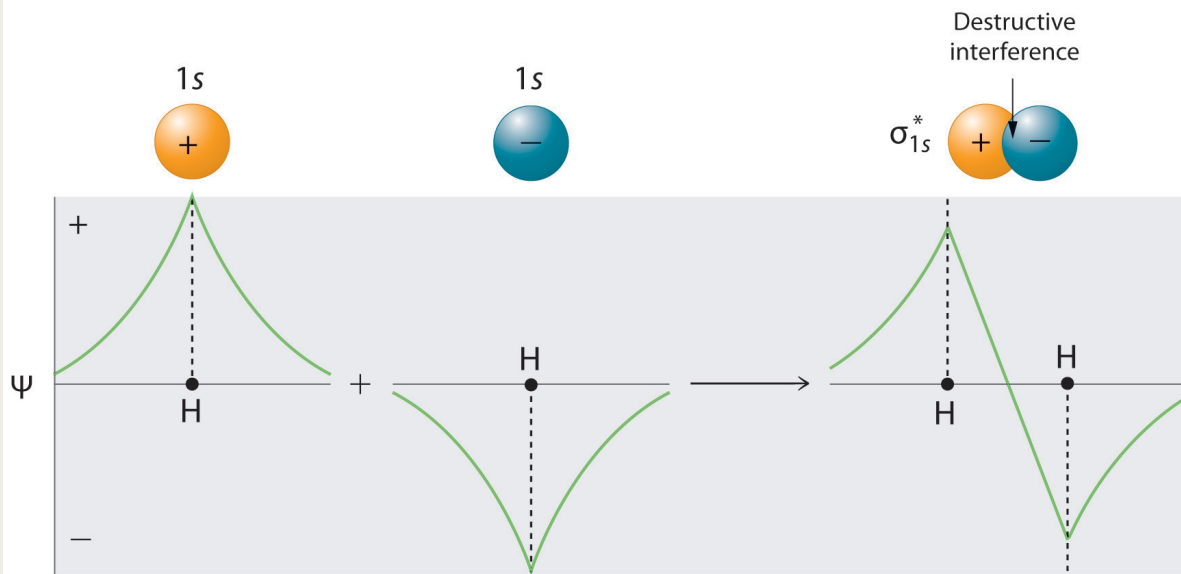
Interference of orbitals in H₂ molecule



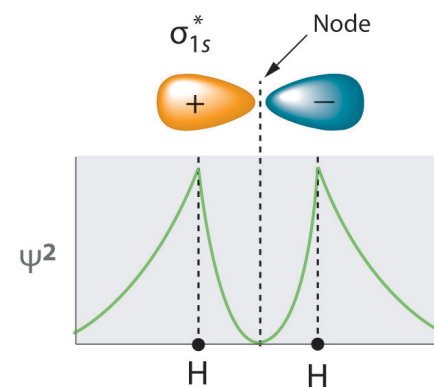
(a) Wave functions combined for σ_{1s}



(b) Bonding probability density



(c) Wave functions combined for σ_{1s}^*



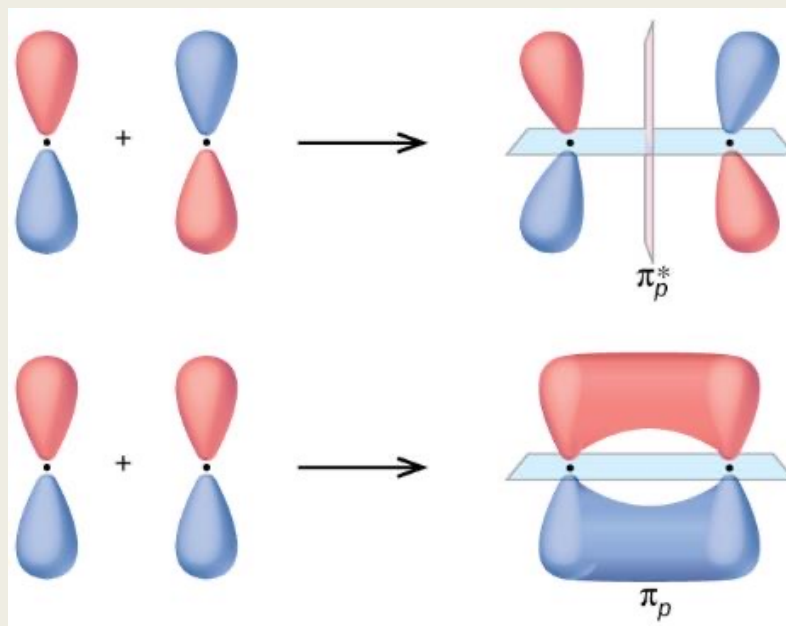
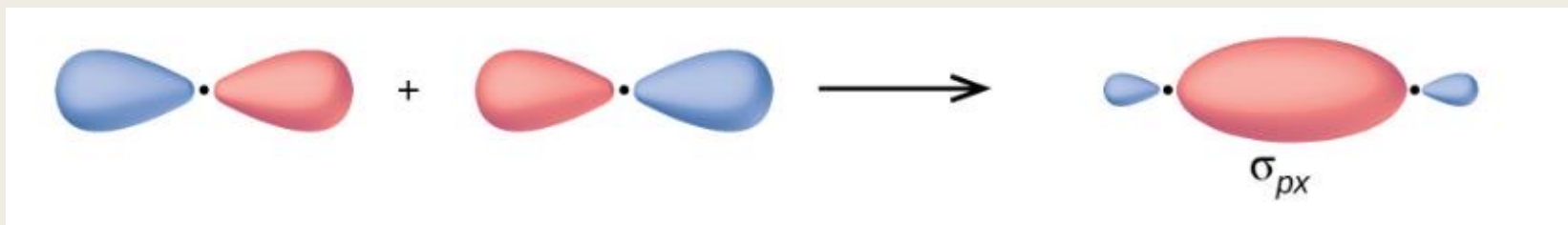
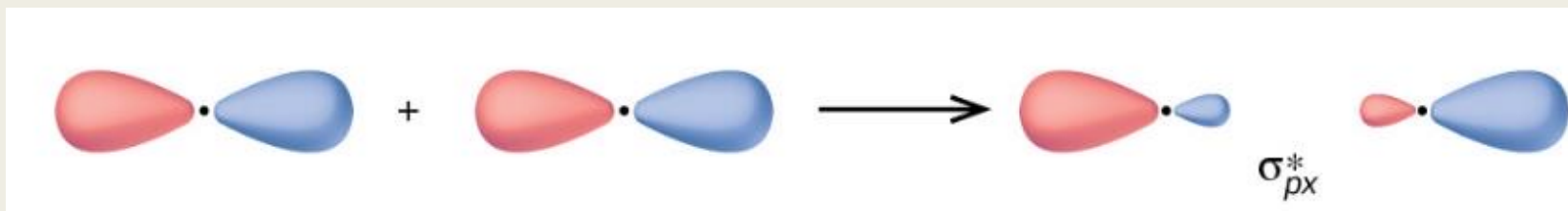
(d) Antibonding probability density

H_2 vs H_2^-

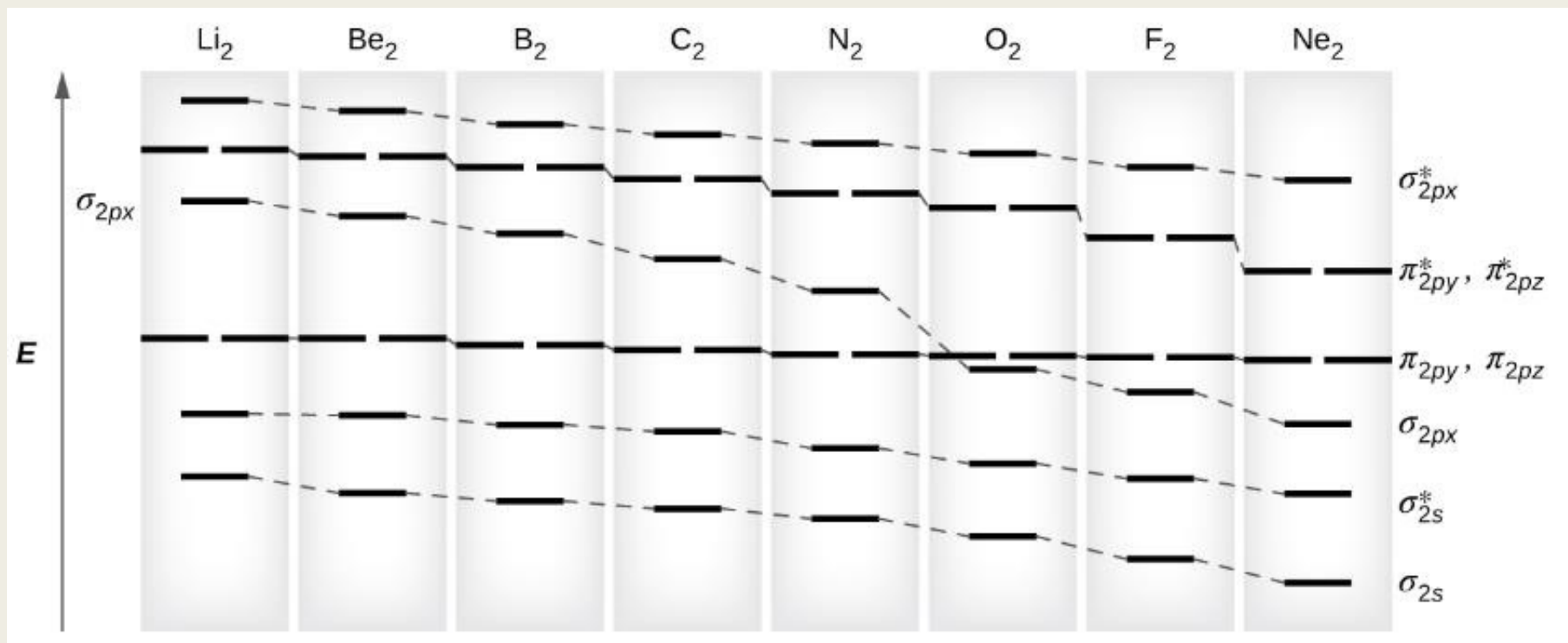
Would the bond length be longer or shorter in H_2^- relative to the bond length in H_2 ?

Would the bond dissociation energy be greater or smaller in H_2^- relative to H_2 ?

Interference with p-Orbitals

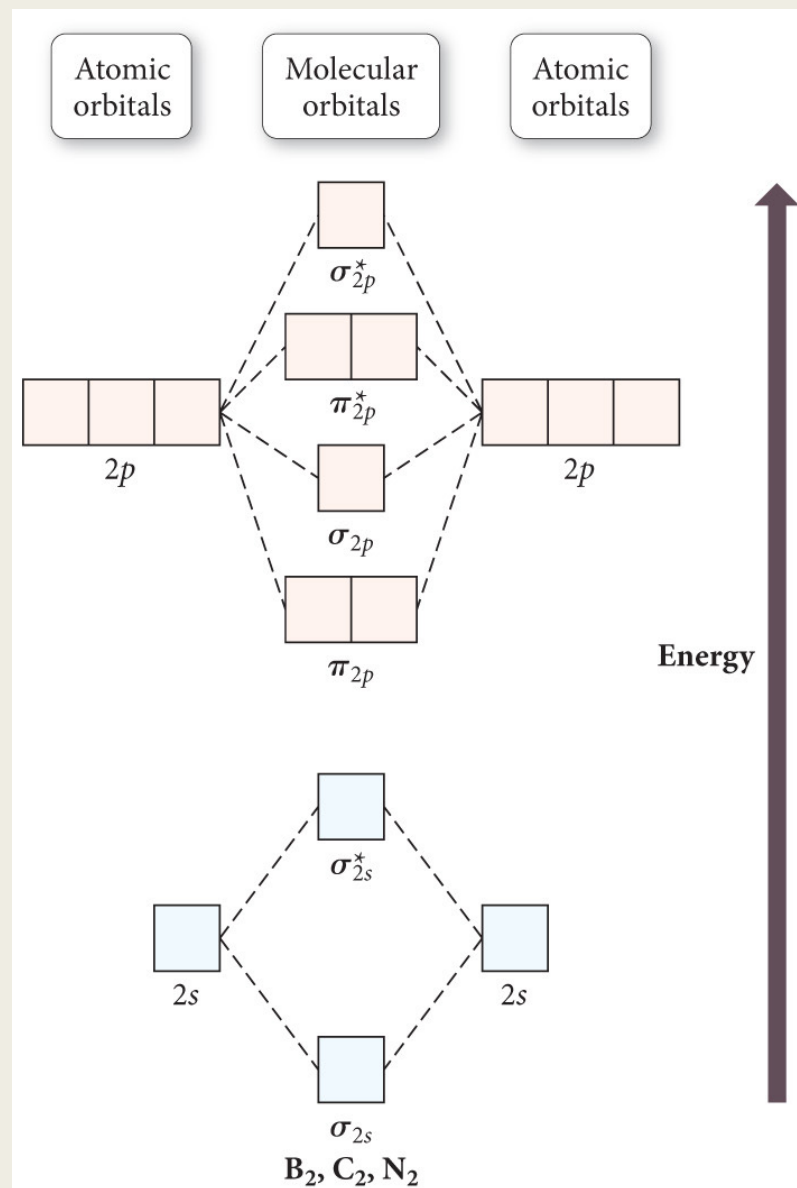
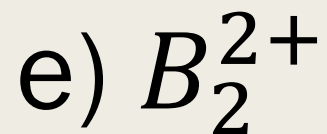
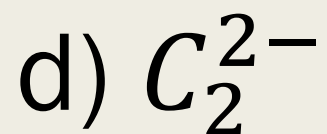
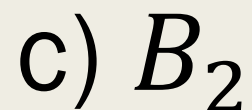
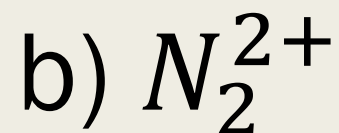
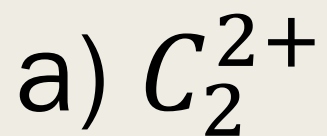


Molecular Orbital Diagrams for Homonuclear Diatomic Molecules



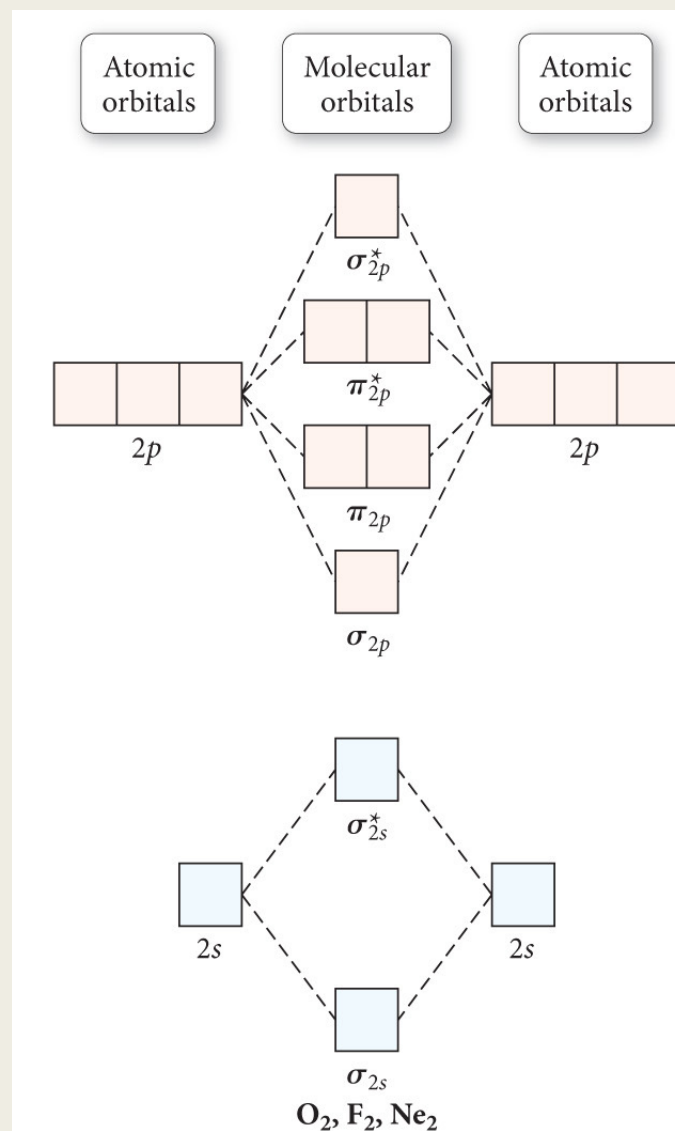
The orbital energies decrease across the period as the effective nuclear charge increases and atomic radius decreases. Between N_2 and O_2 , the order of the orbitals changes.

Draw the molecular orbital diagram to determine which of the following is most **stable**



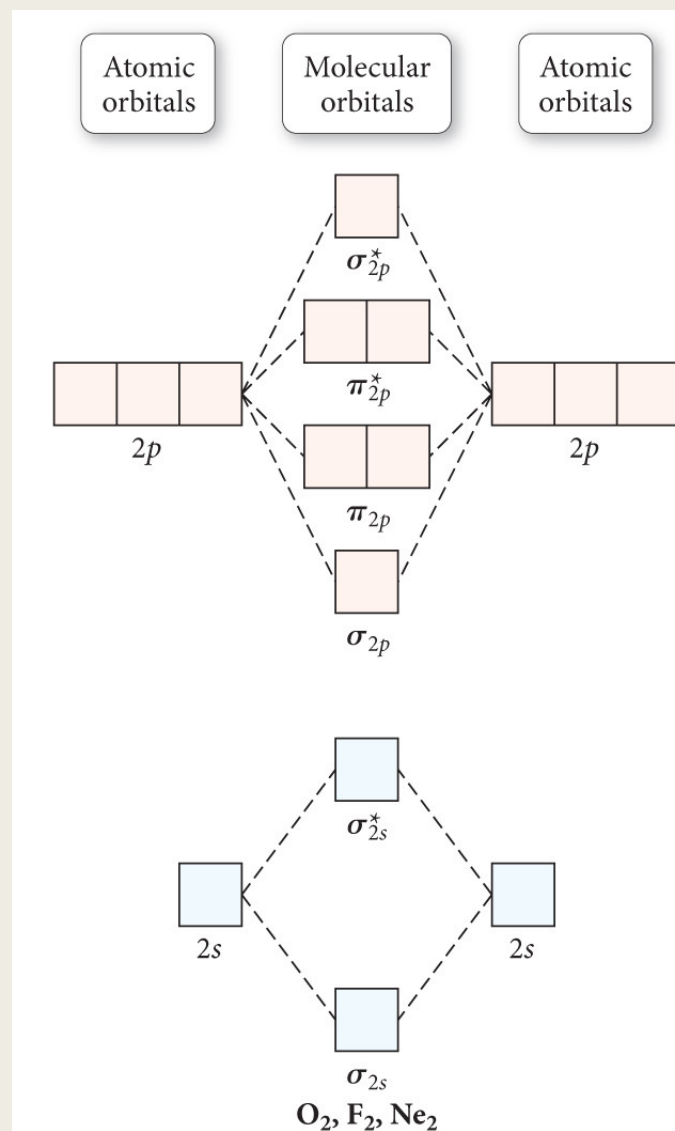
What is the bond order for F_2 ?

- a) 2
- b) 1.5
- c) 1
- d) 0.5
- e) 0



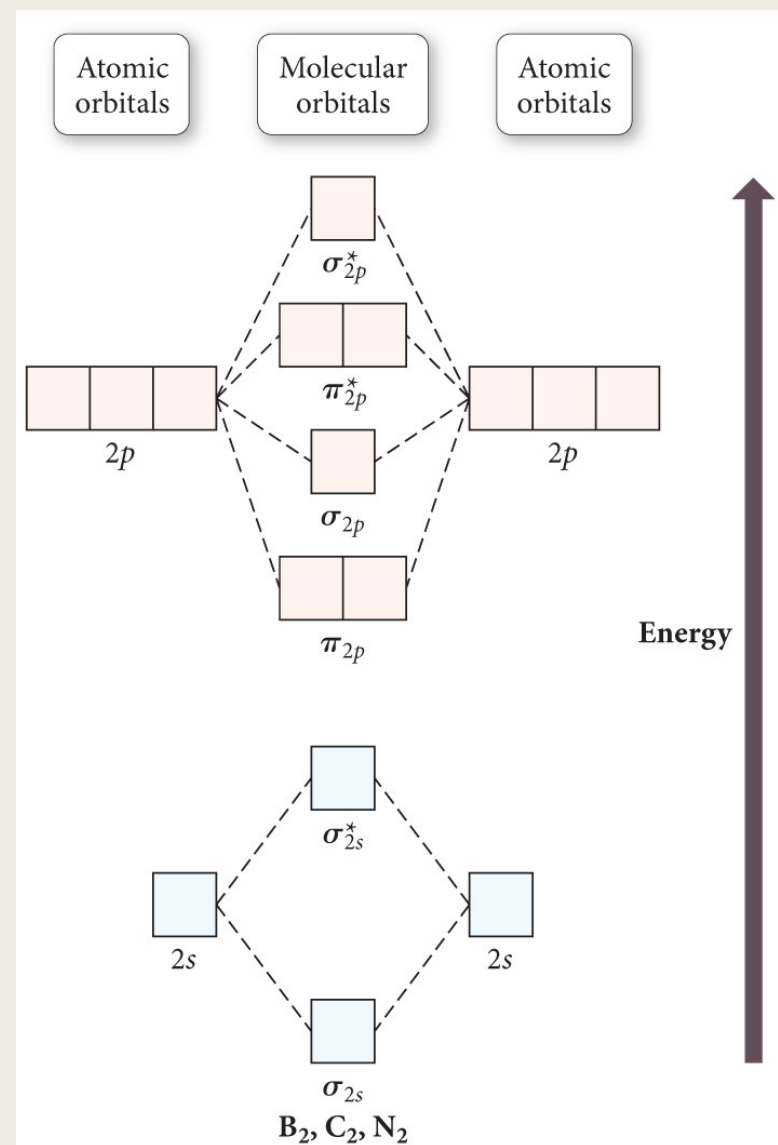
What is the bond order for F_2^+ ?

- a) 2
- b) 1.5
- c) 1
- d) 0.5
- e) 0



According to MO theory, which of the following has the shortest bond length?

- a) C_2
- b) C_2^+
- c) C_2^-
- d) All are the same.
- e) This cannot be determined from the information given.



Molecular Orbital Theory Application

BN, boron nitride, has been used for a variety of applications because of its physical and chemical properties. Namely, BN is quite stable at very high temperatures. Answer the following questions related to BN.

- a) Draw a Lewis structure for BN
- b) Draw an MO diagram for BN
- c) Is BN paramagnetic or diamagnetic?

Consider CO and CN⁺. Use MO theory to answer the following:

- a) Which is more stable?
- b) Which has a longer bond?
- c) Which has a smaller ionization energy?
- d) Is either structure paramagnetic?

A stable molecule has more electrons in _____ orbital than in _____ orbital.

- a) a bonding; an antibonding
- b) an antibonding; a bonding
- c) a molecular; an atomic
- d) an atomic; a molecular

Molecular Orbital Theory Summary

- The simplest molecular orbitals are linear combinations of atomic orbitals (LCAOs), weighted averages of the atomic orbitals of the different atoms in the molecule.
- When two atomic orbitals combine to form molecular orbitals, they form one molecular orbital of lower energy (the bonding orbital) and one of higher energy (the antibonding orbital).
- A set of molecular orbitals is filled in much the same way as a set of atomic orbitals (lower energy first, also unpaired electrons, then paired when orbitals are degenerate).
- The stability of the molecule and the strength of the bond depend on the number of electrons in bonding orbitals compared to the number of electrons in antibonding orbitals.



KINETICS!

Rates of Reaction



$$\frac{\Delta NO}{\Delta t} = \frac{[NO]_{final} - [NO]_{initial}}{t_{final} - t_{initial}}$$

