

Announcements

- Final is Tues, Dec 9 3:30 to 5:20pm
- You should expect an exam approximately the same length as the two others (4-5 pages, 16-20 questions)
- Everything to date has been posted-please check. The last day/time to challenge is Dec 9 at 12noon
- There will be one more update-probably Monday for today's quiz and any other BH cycle submissions
- I will be on campus 9-3:30 on Monday and will arrive around 9am on Tues for last minute questions. Use email in between.
- I anticipate that the exams will be graded and grades submitted on about Mon, Dec 15.
- Final exam scores will be posted, per usual, but letter grades will not be.

Information which may be useful

- Exams 1 and 2 will provide the material for 2/3 of the final. The remaining 1/3(approx) will be from chapters 6 and 7. A quiz compilation has been posted. Also, nomenclature, including Stock will be tested thoroughly
- Topics of note
 - Chapter 6
 - descriptive chemistry know general reactions and methods of preparation of the elements.
 - Understand trends in IE and EA
 - Be able to prepare a properly formatted and labeled BH cycle
 - Chapter 7 (much more here)
 - Understand the nature of the covalent bond
 - Be able to sketch the types of σ and π bonds shown in class
 - Be an absolute expert in drawing Lewis Structures, including molecules which are exceptions to the octet rule
 - Understand formal charge and resonance
 - Understand electronegativity and bond polarity and molecular polarity
 - Be able to use VSEPR to produce 3D reps of molecules and to apply the correct geometric label to an atom in a Lewis Structure
 - Understand and use the concept of hybridization, be able to sketch the general shape of an sp hybrid

Hybridization, structures and labels

- The need for hybridization arises directly from observed phenomena such as the tetrahedral nature of CH_4 .
- Likewise VBT and MO theory result from the need to explain observed properties of molecules and bonds

Hybrids and unhybridized p orbitals



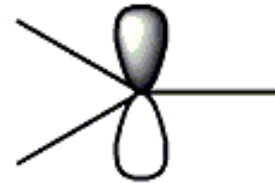
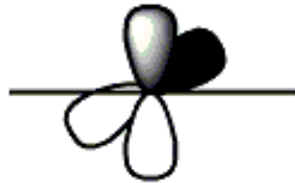
sp-linear



sp²-trig planar



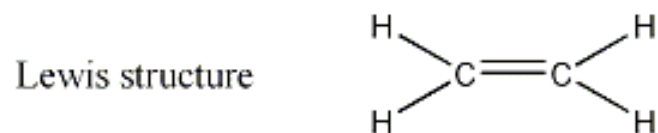
sp³-tetrahedral



The unhybridized p orbitals are perpendicular to the hybrids

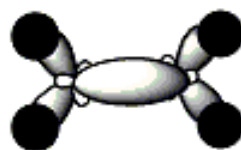
Molecules, bonds and orbital clouds

Representing a molecule with orbital clouds, C_2H_4

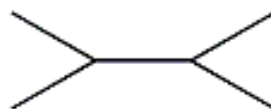


Cs are sp^2 hybridized

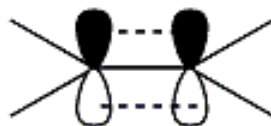
Draw the sigma bonds as overlaps



Redraw the sigma bonds as lines

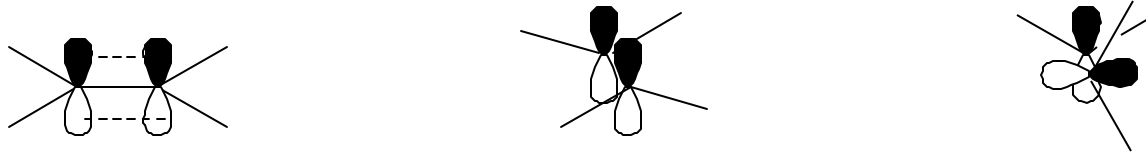


Represent the pi bond(s) as edge wise p overlaps



Impact of pi bonding

- Restrictions on Rotations-the side to side overlap of the p orbitals would be broken if there was rotation about the internuclear axis.

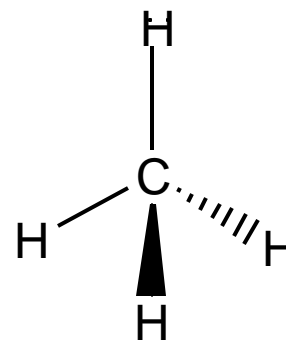
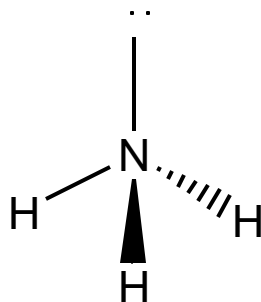
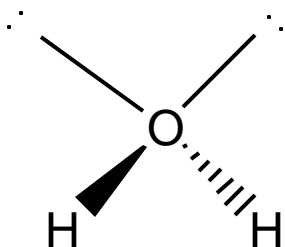


- Planarity-the relative positions of the p orbitals and the hybrids result in the six groups involved in a double bond all being in the same plane

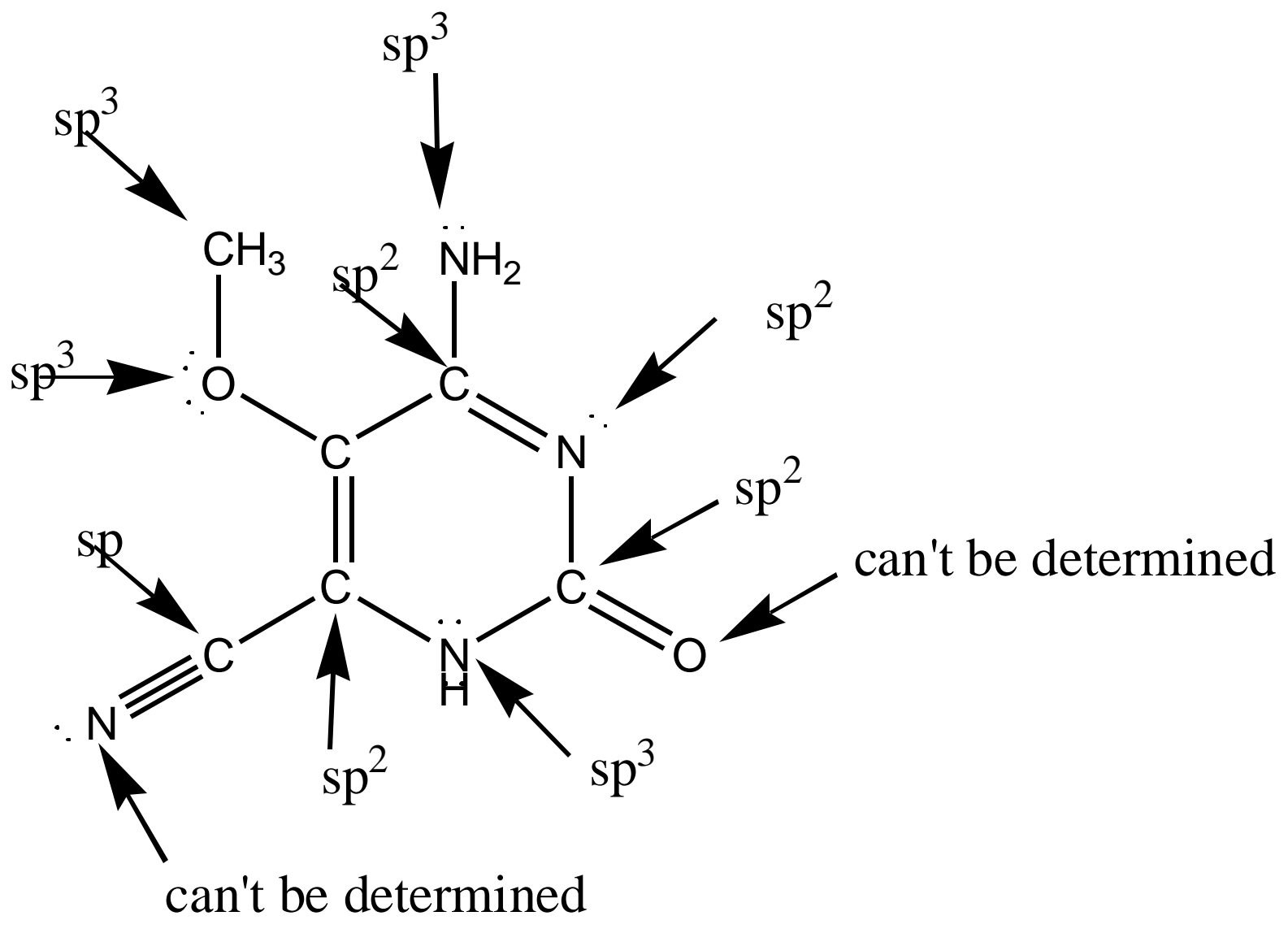


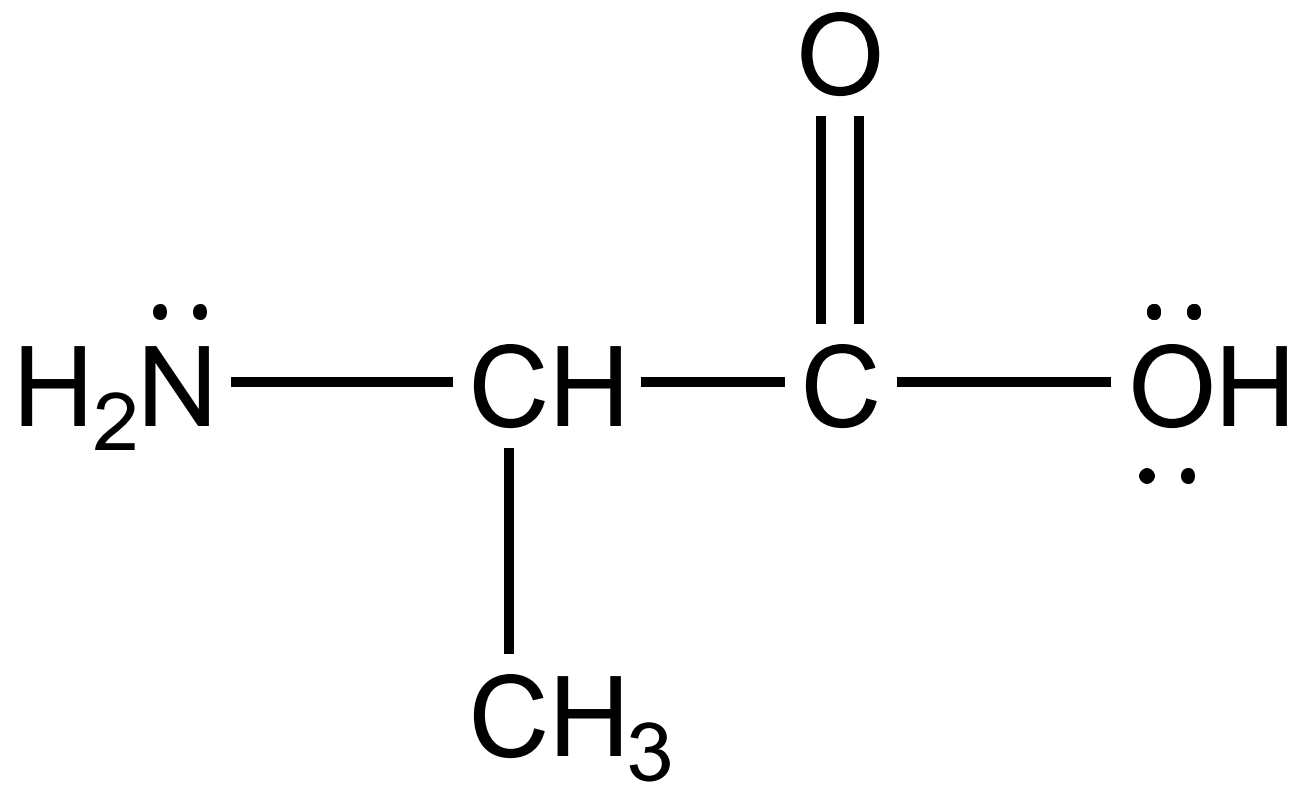
Hybridization and geometric labels

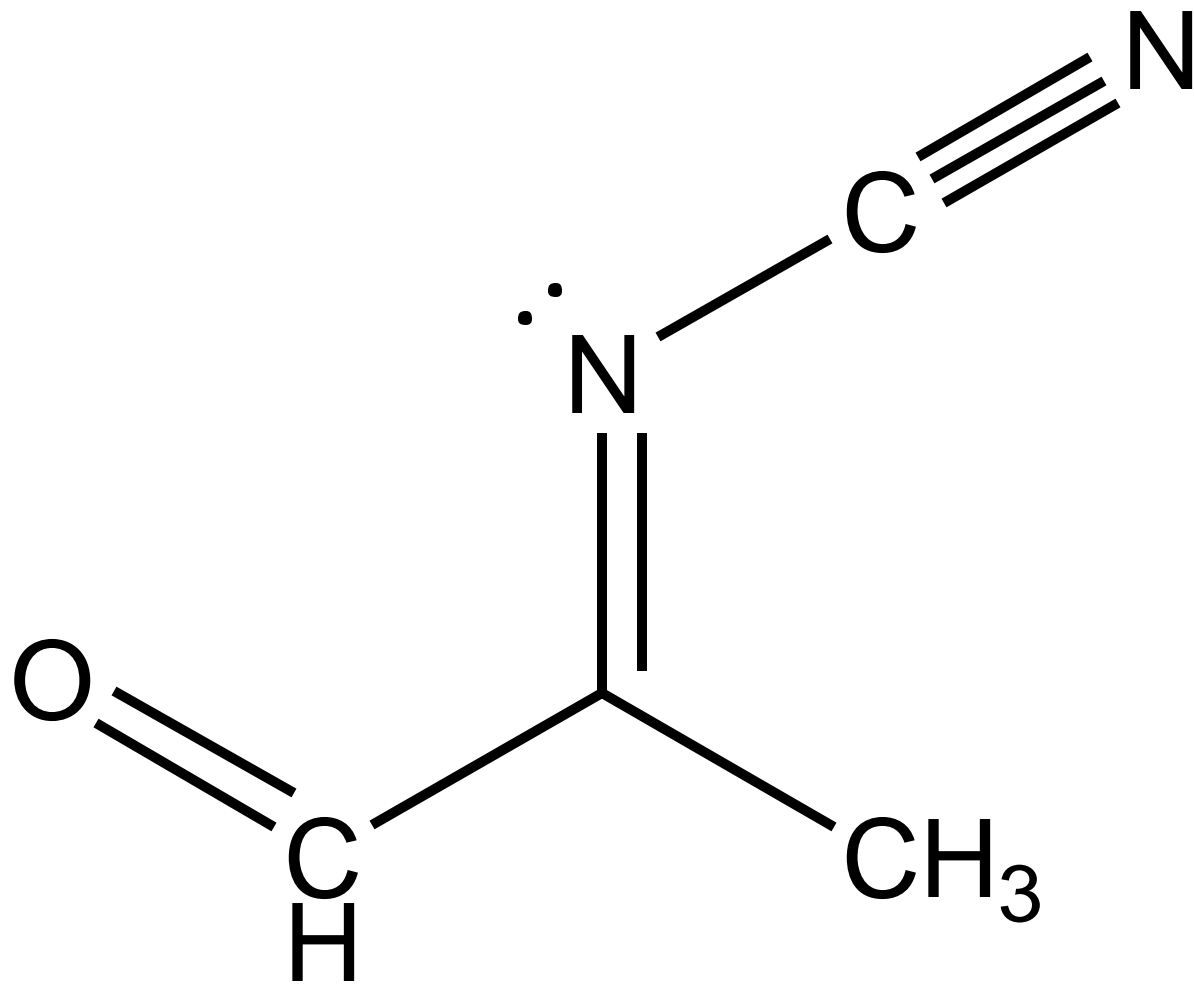
- Hybridization is usually determined by the use of known properties of elements and/or information about a specific compound. One needs to be aware that simple sp type hybrids are much more prevalent before Ne in the periodic table and that hybridization involving d orbitals occurs readily after that point.
- Hybridization should not be claimed for terminal elements or any other elements bound to a single atom.
- Geometric labels are based upon atom positions, not the hybridization. Example: H_2O (AX_2E_2), NH_3 (AX_3E), CH_4 (AX_4) are all sp^3 hybridized but are labeled: bent, trigonal pyramid and tetrahedral based upon the atom positions

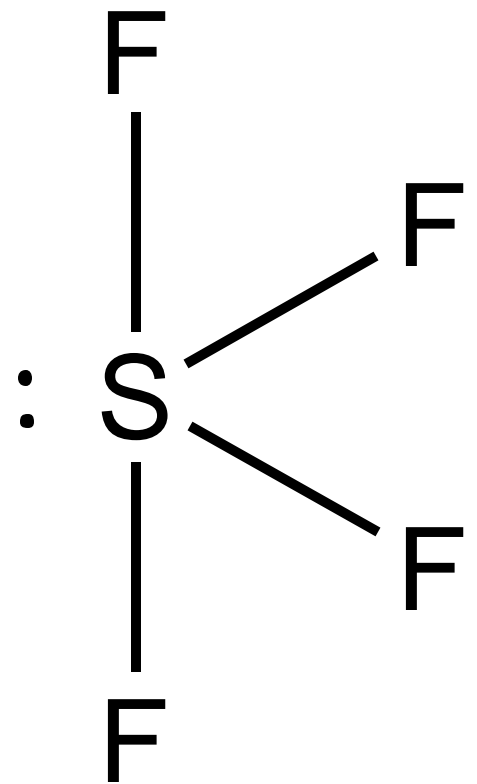
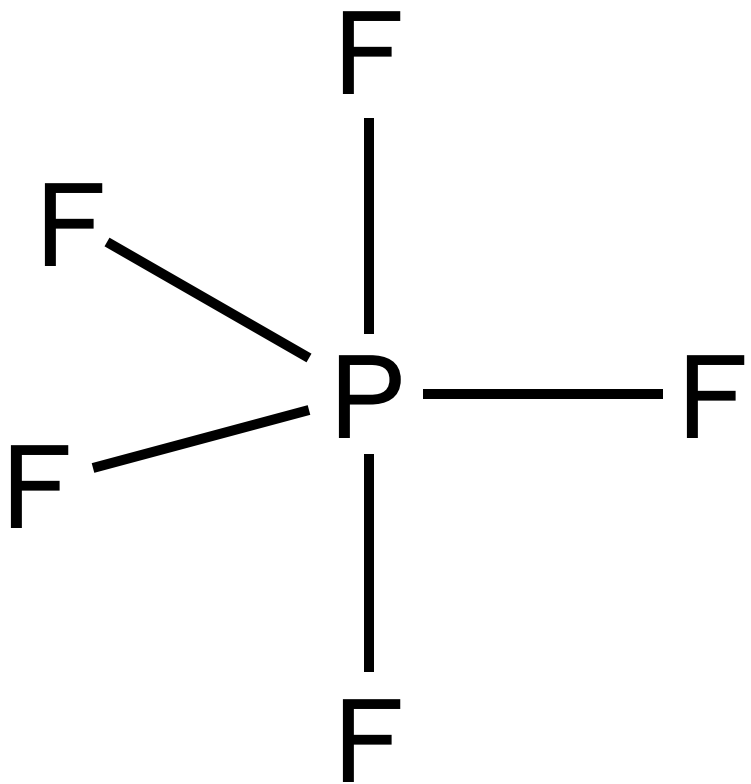


..



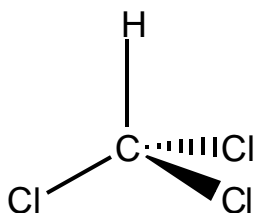






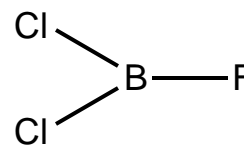
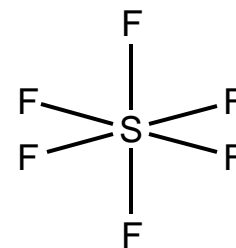
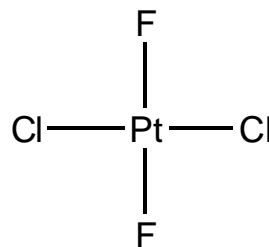
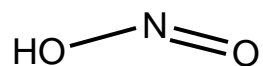
Molecular Polarity

- Differences in electronegativity produce polar bonds.
- Overall molecular polarity results from the combination of the individual bond polarities.
- Molecules can be nonpolar, even if they have polar bonds, if the bonds cancel out. ex: CO_2 , CCl_4
- Which of the following would you expect to be polar?



CS_2

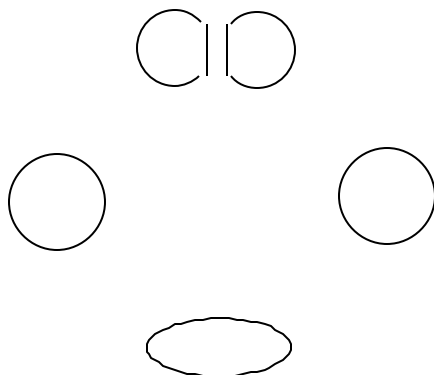
HCN



Molecular Orbital Theory

- The representation of sigma and pi bonds as orbital overlaps reinstates the view of electrons as occupying volumes of space rather than specific positions which Lewis dot structures indicate
- A volume of electron probability which extends over two or more atoms is called a molecular orbital and is to a molecule what an atomic orbital is to an atom.
- Molecular orbitals are produced by what are termed linear combinations of atomic orbitals (basically adding and subtracting them)

- Each pair of orbitals combined produces a bonding and antibonding MO



- The bonding MO is lower energy than the atomic orbitals, while the antibonding is higher energy. This is because the antibonding has a nodal plane between the nuclei and thus does not effectively screen the nuclear charges from each other
- The sketch of an antibonding orbital looks like a bond orbital with a void(node) between the atoms

Making H₂

_____σ*(antibonding)

Ha(1s)

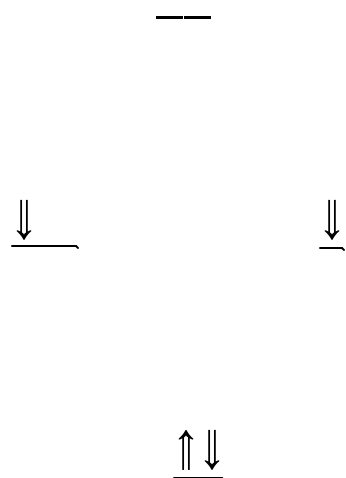
Hb(1s)

_____σ(bonding)

H₂

Filling MOs

- The production of a molecule results in the conversion of the valence atomic orbitals into molecular orbitals. All of the valence electrons must then be “moved” to the Mos following the same rules used for the filling of atomic orbitals. In making H_2 , the two electrons are placed in an MO which is labeled σ_{1s} .

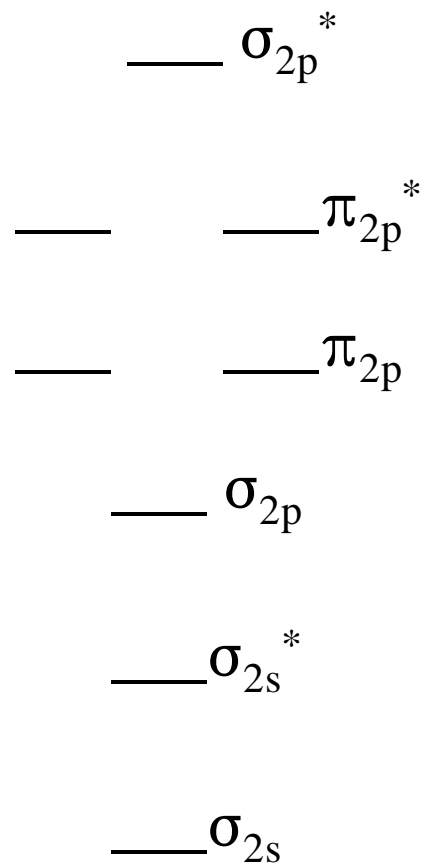


Information from MO Diagrams

- Bond order:
 $\frac{1}{2} * (\text{Bonding e-s} - \text{Antibonding e-s})$
- Diamagnetic or paramagnetic:
 - diamagnetic-no unpaired electrons
 - paramagnetic- one or more unpaired e-s
- Why compounds do/don't exist

General MO Diagram

- See text page Fig 7.18(p282) and 7.20(p283)



Filling this diagram is in precisely the same fashion as filling an atomic orbital diagram