

Chem 107B – Structure of Atoms

1. Each group is to talk about your current knowledge of the structure of atoms. Some things you might consider include:

What important fundamental particles make up atoms?

Do these particles have charges? If so, what are the charges?

How are those particles arranged in atoms?

Suppose you had to explain what an atom looked like to a 10 year old. Draw a picture that would help in your explanation.

Are there any things you simplified in your picture?

Chem 107B – Structure of Atoms, Part 2

1. Now that we know that atoms have electrons, protons, and neutrons, how could we visually represent each of these?
2. Before the nuclear picture of the atom, what picture was used to visualize the structure of an atom?

Aside: We need to understand the experiment of Thompson in 1897 to measure the mass-to-charge ratio of an electron and the experiment of Millikan in 1909 to measure the charge of an electron (thereby enabling the mass of an electron to be calculated).

3. Devise an experiment that would lead to the conclusion that atoms had a nucleus.

Hint: Think of trying to show, perhaps in the dark, and without moving from a single spot, whether a barrier in front of you was made of a very thin mat of cotton or mostly of air with some hard, metal disks.

What are the differing observations that would allow you to distinguish the nuclear picture (some hard, metal disks) from the cotton mat?

Chem 107B

BLACKBODY RADIATION

1. A heated object (e.g., iron rod in a hot flame) glows. What process occurs at the molecular or atomic level inside the rod that could account for the emission of light?
2. Suppose you passed the emitted light through a prism and recorded the intensity of light at each specific wavelength. Draw what you might observe as a plot of the intensity (y-axis) versus wavelength (x-axis). For convenience sake, you might just show an x-axis that has ultraviolet, visible, and infrared labeled from left to right on the axis.

PHOTOELECTRIC EFFECT

1. The following observation was made at the turn of the century.

Light, when shined on a metal surface, causes the emission of electrons from the metal. Apparently, the light energy is sufficiently large to pull a negatively charged electron away from the positive matter of the atom.

Remember, at this time there was not an accurate image of what the atom looked like. The presence of electrons was accepted, so people knew that there must be some positive matter, but the nuclear picture was not known. Fortunately, the observation can be understood no matter what the picture of the atom, so long as it is appreciated that the electron is negative and that positive matter is present.

However, different metals exhibit different properties. Some metals give off electrons when illuminated using an ordinary light bulb. Other metals do not. For the metals that do not give off electrons using one ordinary light bulb, what might you change about your experimental conditions in an attempt to see when and if electrons will be given off?

Hypothesize what you might observe when making the changes you propose.

Chem 107B – Introduction to Global Warming

Discuss what you would like to know about global warming. Also discuss what you already know about global warming. Things to consider in your discussion include:

1. What chemicals and processes cause it?
2. Is anything being done about it?
3. What do/don't we know about global warming?
 - Is it actually happening?
 - What are the consequences, if it is?

Chem 107B - Discussion Topics - Global Warming

1. What is your opinion regarding whether emissions of carbon dioxide and other greenhouse gases should be reduced?
2. Would you support initiatives to undertake global climate engineering?
3. Should developing countries have to participate in greenhouse gas emission reduction programs?
4. Should the US implement a tax on the cost of new cars related to their fuel efficiency?

The following scheme has been proposed:

Over 50 mpg - no tax
40-50 mpg - \$1,000 or 5% of the cost of car (whichever higher)
30-40 mpg - \$2,000 or 10% of the cost
20-30 mpg - \$3,000 or 15% of the cost
10-20 mpg - \$4,000 or 20% of the cost
0-10 mpg - \$5,000 or 25% of the cost

5. The issue of global warming is so complex that we will never have a computer model that will predict future environmental consequences with absolute certainty. Given that, we could ask whether additional science mostly confuses the issue and paralyzes us from acting.

There is certainty that carbon dioxide levels are rising and consumption of fossil fuel is the primary cause. One could then argue that the environment must respond to this change in some way, and that we as humans, even if we cannot possibly understand the consequences, have an obligation to minimize this change.

Which position would you take? One is that we continue to refine the science and our understanding before taking significant action on global warming. The other is that we act now to mitigate the possibility of changes that might or might not occur.

Chem 107B – Electronic configurations

1. Write the electronic configuration for carbon (element 6).

Consider the last two electrons in the carbon configuration. Do you see how there are two different ways in which the electrons could be situated? Make sure you understand the difference between the two ways.

It is possible to measure whether an atom has unpaired electrons or not. Atoms with unpaired electrons interact with a magnetic field whereas those with all the electrons paired do not. By measuring the specifics of the interaction with the magnetic field, it is even possible to determine the number of unpaired electrons in an atom. For carbon, it has been determined that each atom has two unpaired electrons. Does this agree with one of the possible configurations?

NOTE: Atoms or molecules with unpaired electrons are said to be **PARAMAGNETIC**. Those with all the electrons paired are said to be **DIAMAGNETIC**.

Use the information observed with carbon to develop a generalization for the filling in of electrons into orbitals with the same energy. This generalization holds all the time and is referred to as the Aufbau principle.

2. Write the electronic configuration for chromium (element 24).

Experiments on chromium show that it is paramagnetic. Does this agree with your configuration? How many electrons are unpaired in your configuration?

The measurements also show that chromium has six unpaired electrons? Explain how you could arrive at an electron configuration for chromium that has six unpaired electrons.

What does the configuration for chromium that is actually observed in nature suggest about the relative stabilities of certain electronic configurations?

Chem 107B - Worksheet on Electronegativity, Ionization Energies, Electron Affinities, and Atomic Radii

1. Electronegativity: The electronegativity expresses how much a particular element wants an electron. The higher the value, the more that particular atom wants an electron.

The following page has a periodic table that lists the electronegativities of each element. The absolute values do not have meaning. What does have meaning is the relative values. Note that the noble gases (He, Ne, Ar, ...) are not included since these elements have stable configurations and do not want to gain electrons.

A) Examine the electronegativities of the halogens (F, Cl, Br, and I). Is there a trend? If so, propose an explanation that would justify the trend.

B) Examine the electronegatives for the period that includes the elements lithium (Li) through fluorine (F). Is there a trend? If so, propose an explanation that would justify the trend.

2. First Ionization Energy: This refers to the energy that is needed to remove one electron from an atom. The remaining substance would therefore have a charge of +1.

The plot on the next page lists shows first ionization energies as a function of atomic number. Note that all the values are positive since it always takes energy to pull an electron away from the positive nucleus of an atom. The larger the number the more difficult it is to remove the electron.

A) Examine the plot for the series going from lithium to neon (it might be useful to look at a periodic table at the same time to see where these elements are).

What is the general trend that occurs moving across from lithium to neon? Propose a reason that would explain this trend.

There are two breaks in the plot. One occurs between the elements beryllium (Be) and boron (B). Propose a reason why the plot exhibits a discontinuity at this point.

The second occurs between nitrogen (N) and oxygen (O). Propose a reason why the plot exhibits a discontinuity at this point.

Do your explanations for the discontinuities support our current idea that there are such things as s and p orbitals?

B) Examine the values for the halogens (F, Cl, Br, I). Is there a trend in this data? Propose a reason for the trend.

C) It is also possible to measure the second and third ionization energies for elements. These would refer to the energies needed to remove a second and third electron respectively, thereby leaving either a +2 or +3 ion remaining.

The chart below lists some ionization energies for several elements (all are in units of kilojoules/mole).

<u>Element</u>	<u>1st</u>	<u>2nd</u>	<u>3rd</u>	<u>4th</u>
sodium (Na)	495	4560		
magnesium (Mg)	735	1445	7730	
aluminum (Al)	580	1815	2740	11,600

Why is the second ionization energy of magnesium higher than the first?

Why is the third ionization energy of magnesium so much higher than the second?

Explain why there is such a large jump between the third and fourth ionization energy of aluminum.

Do these observations provide additional support regarding our scheme for writing electronic configurations for atoms?

3. Electron Affinity: The electron affinity is measured by effectively “forcing” an atom to gain an electron and assume a charge of -1.

A plot of electron affinities for several elements are given on the next page. If an atom really wants an electron, as it gains one energy might be given off. Such elements would have negative values for their electron affinity. If an atom does not want an electron, it does then have to be “forced” to gain one and would have a positive electron affinity.

Examine the values for sodium (Na) through argon (Ar).

A) Which element in this group has the most positive electron affinity? What would account for this observation?

B) Which element in this group has the most negative electron affinity? What would account for this observation?

C) Compare the values for silicon (Si) and phosphorus (P) and explain the difference between the two.

D) Do these trends lend further support for our current understanding of electronic configurations of atoms?

4. Atomic radius: Because we can never exactly locate the positions of electrons, the atomic radius is something of an arbitrary number for the dimensions of an atom. One way to calculate the atomic radius might be to take a pure piece of a metallic element (say iron for example) and measure the distance between adjacent nuclei. Subtracting this number by two would provide a measure of the radius of each iron atom.

The next page has a plot of the atomic radii for the many atoms in the periodic table.

A) Examine the trend for the elements sodium through chlorine. What is the general trend across this column and propose a reason for the trend?

B) Are there any anomalies in the plot? If so, why do you think these elements vary from the general trend?

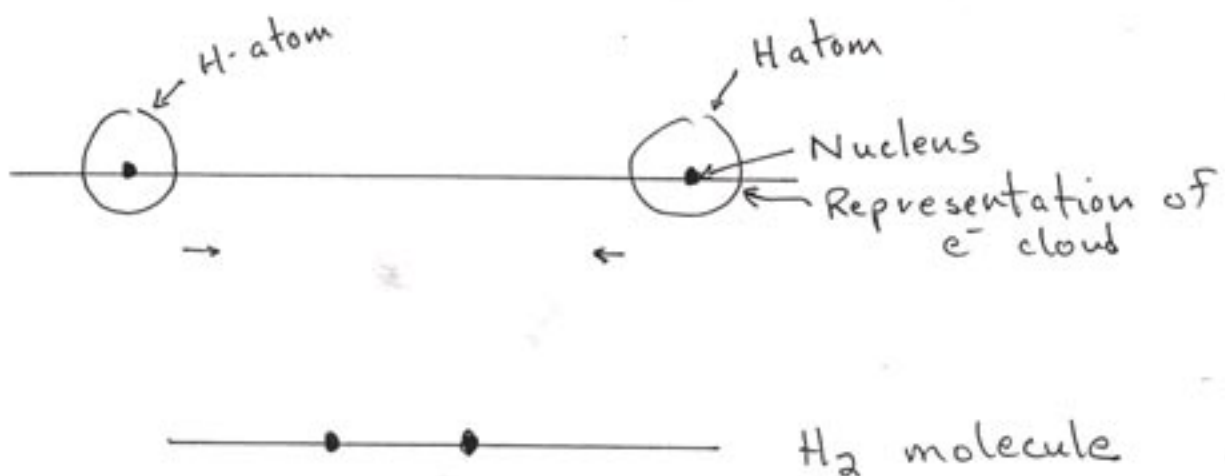
Chem 107B: Molecular Orbitals

Our current picture of atoms involves the understanding that electrons exhibit a wave-particle duality and are found in regions of space called atomic orbitals. Similarly, electrons in molecules are found in regions of space and we can call these regions molecular orbitals. Just like the wave function and energy of an electron in an atom could be solved for using the Schrodinger equation (remember as well that the square of the absolute value of the wave function can be used to show the orbital shape that the electron is in), the wave function and energy of an electron in a molecule can be solved for using the Schrodinger equation. Performing such calculations is an involved process that we will not do in this course.

For some small molecules, however, it is rather straight forward to get a picture of what the molecular orbitals look like by first considering what the atomic orbitals of the component atoms look like. In particular, this method works especially well for a group of compounds referred to as homonuclear diatomics (common examples include hydrogen gas – H_2 , fluorine gas – F_2 , chlorine gas Cl_2 , bromine - Br_2 , and iodine – I_2)- In these examples, **the molecular orbitals simply look as if the atomic orbitals from each of the atoms have overlapped.**

Let's consider what happens for hydrogen gas as an example. In this case, each of the hydrogen atoms has its one electron in a 1s orbital. The pictures below represent two hydrogen atoms and each shows a representation for the 1s orbital. In this case the two atoms are far enough apart so that they do not interact to form a bond. Now consider bringing the two atoms close enough together so that their atomic orbitals overlap.

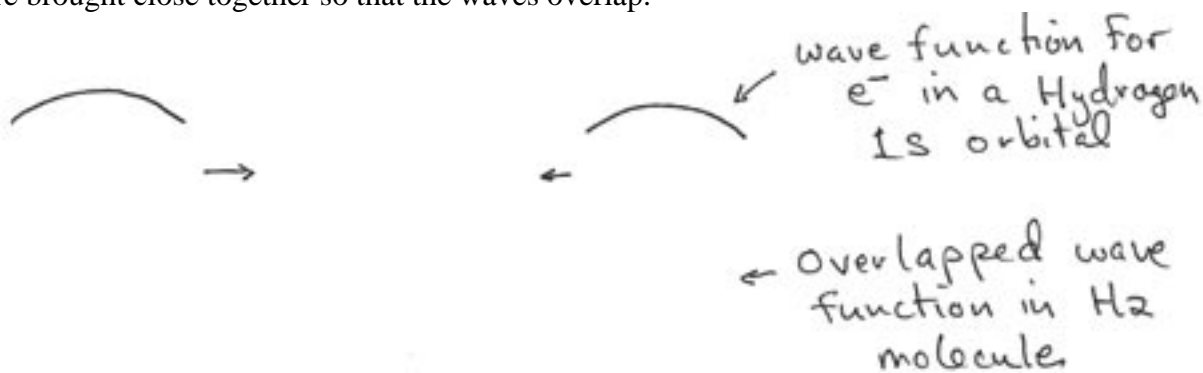
In the center draw what you think the molecular orbital that would result from the overlap of the two atomic orbitals would look like.



Another way to think of this is that the wave function of an electron in a molecule is a sum of the

wave functions that describe the electrons in the atoms. Representations of the wave functions of the electrons in each of the hydrogen atoms are shown below (NOTE: The representations might not look like a typical wave. In this case they are essentially half of one complete wave.)

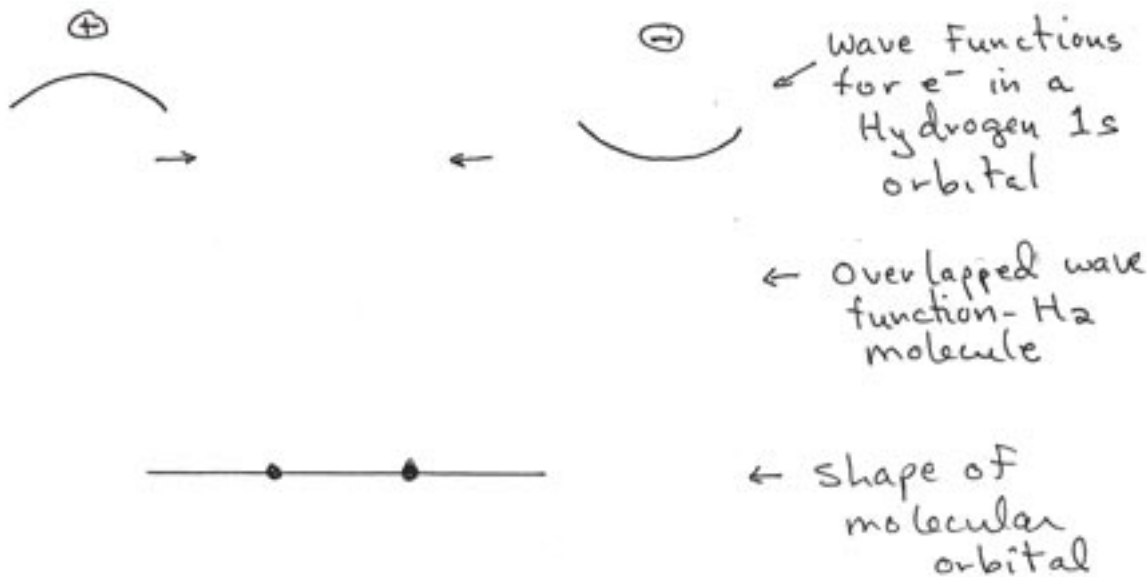
Draw in the center the resulting wave function of the electron in the molecule as the two atoms are brought close together so that the waves overlap.



Remember that the orbital shape is the square of the absolute value of the wave function. Would the square of the wave you have drawn above look like the orbital you drew on the previous page?

Note that so far we have combined two atomic orbitals with the result of getting one molecular orbital. **It turns out that if two atomic orbitals are overlapped in a molecule, two molecular orbitals must result.** The second molecular orbital is obtained by combining the two wave functions shown below. Note that now the wave functions have the same shape, but differ in the signs of their amplitude (one has positive amplitude, the other negative).

Draw in the center the resulting wave function of the electron in the molecule as the atoms are brought close together. Below that, draw what this molecular orbital would look like.



Below are shown the two molecular orbitals in hydrogen gas that result from the overlap of the two 1s atomic orbitals of hydrogen.



Two molecular orbitals in the H_2 molecule.



From overlap of 1s orbitals.

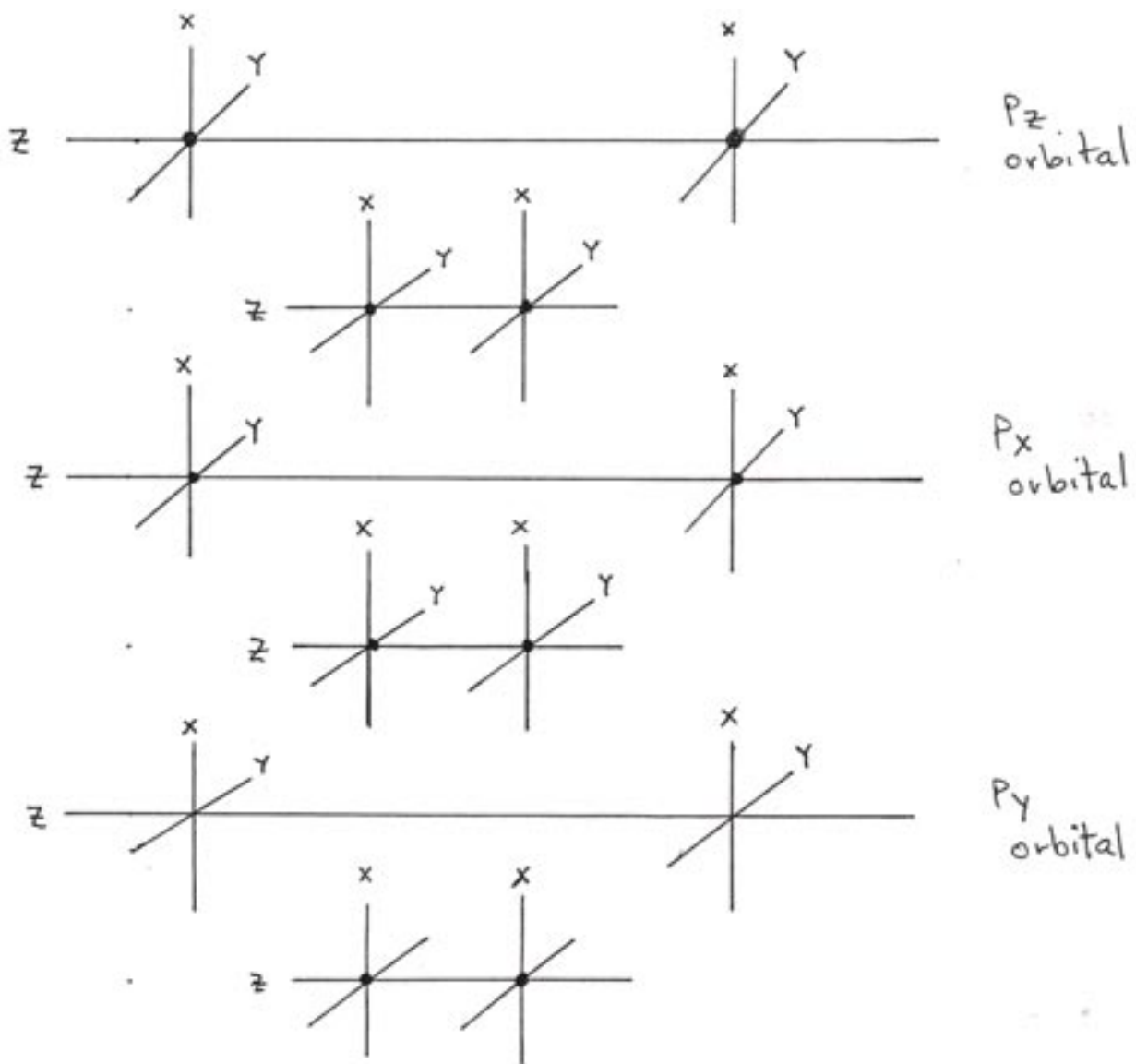
Note that the top one locates most of the electron density between the two hydrogen nuclei, and that the bottom one locates most of the electron density outside of the two nuclei. One of these orbitals is referred to as a **bonding orbital**, the other as an **antibonding orbital**.

Which of the two above do you suppose is the bonding orbital?

Do you think these two molecular orbitals have the same or different energy?

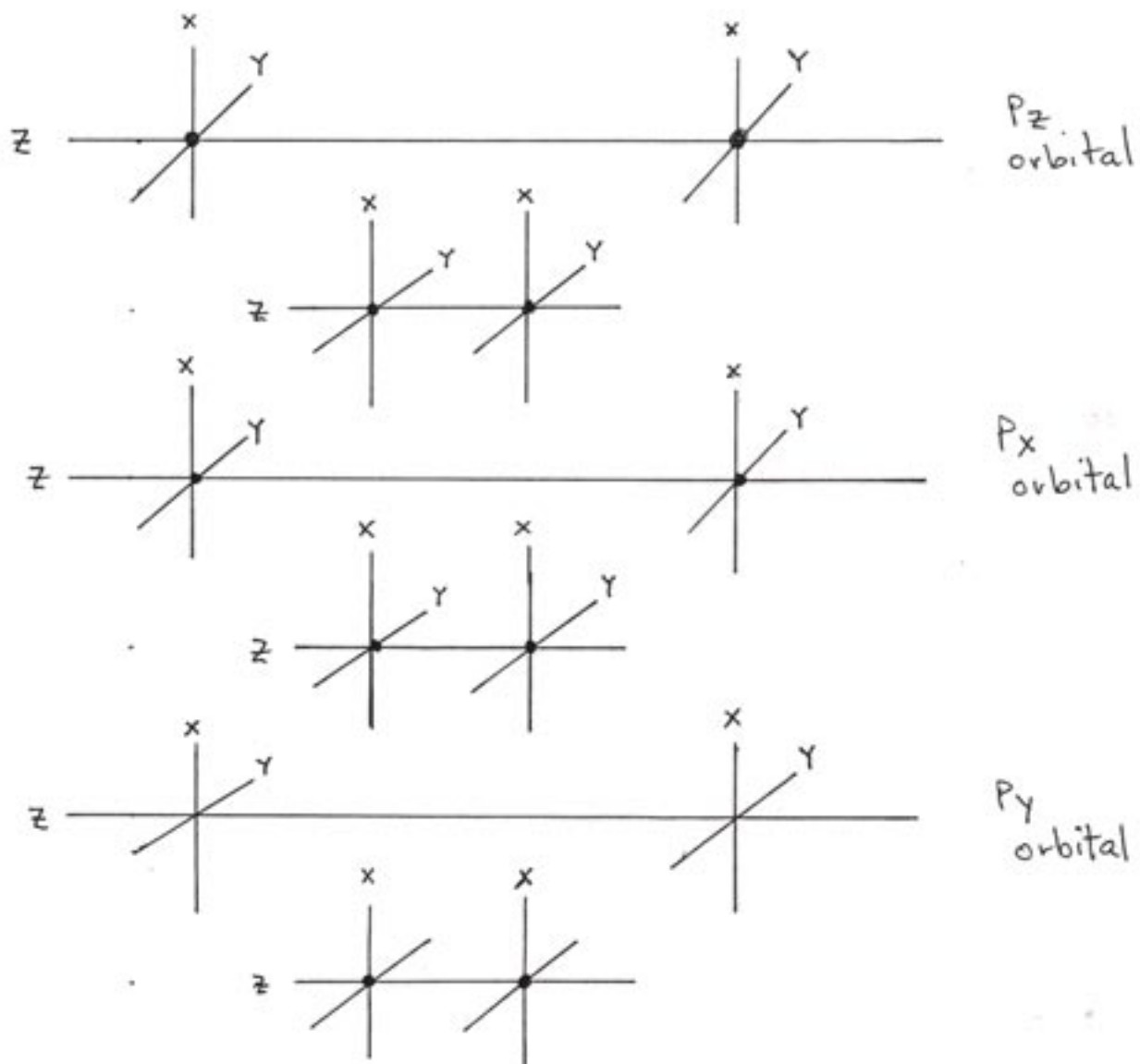
If different energy, which one do you think is lower in energy (remember, the one lower in energy will fill in first with electrons).

A similar set of pictures would result if we combined atoms that had electrons in the 2s orbitals, except that the molecular orbitals would be bigger in size than those that resulted from the overlap of the 1s orbitals. Overlapping the 2p orbitals is different, though, because the p-orbitals have different orientations in space. By convention, both atoms that are overlapping have the same z-axis. On the sets of axes shown below, first draw in the p_x , p_y , and p_z orbitals where labeled. Below each set of atomic orbitals, draw a representation for the bonding orbital (positive overlap of the wave functions) that would result as the atomic orbitals are overlapped with each other.



Do you see any difference in the bonding orbitals that result? Explain.

Repeat the same process below except now draw in the antibonding orbitals (negative overlap of the wave function) that would result.



We have a convention for naming molecular orbitals.

Bonding orbitals with **one region of overlap** are referred to as σ (sigma). The corresponding antibonding orbital is denoted as σ^* .

Bonding orbitals with **two regions of overlap** are referred to as π -orbitals (pi). The corresponding antibonding orbitals are denoted as π^* .

Out-of-class assignment: Molecular Orbitals

Draw the corresponding bonding and antibonding orbitals that would result from the overlap of the d-orbitals. The section in your book on atomic orbitals shows good pictures of what the d-orbitals look like that you will need to complete the assignment.

Some reminders and hints.

- 1) Remember that the two atoms have the same z-axis and that the x- and y-axes of each atom are parallel to each other (refer back to the p-orbital picture to see how the axes align).
- 2) Do not worry about the donut portion of the d_{z^2} orbital. This part will not get involved in any overlap and can be ignored.
- 3) Name the resulting orbitals. Remember, molecular orbitals with one region of overlap are σ -orbitals, two regions are π -orbitals.
- 4) If you get any with more than two regions of overlap, we have not learned the name for those yet.

By the way, this is not merely an academic exercise to see if you can draw how atomic orbitals overlap to form molecular orbitals. In certain transition metal complexes there are metal-metal bonds. These metal-metal bonds involve the formation of molecular orbitals from overlap of the d atomic orbitals.

Chem 107B: Lewis Structures

Write Lewis structures for the following compounds. In each case, write all possible resonance forms and decide on the basis of assigned formal charges whether any form(s) are preferred over others.

1. Carbon dioxide – CO_2

2. Ozone – O_3

3. Nitrous oxide – N_2O

4. Nitrogen dioxide – NO_2

5. Sulfuric acid – H_2SO_4

Chem 107B: Molecular Shape (Geometry)

1. Consider a molecule with:

- an atom C in the center
- two atoms of A bonded to C

If we wanted to describe its MOLECULAR SHAPE (in other words, some description of the relative location of the atoms in space), what parts of the molecule would we need to know the relative spatial locations of?

2. There are only two general ways that the nuclei of a three-atom molecule such as the one above can be configured. What are those two ways?

3. What in a molecule do you think impacts the spatial positioning of the nuclei?

4. Thinking about Lewis structures, in what ways do electrons show up about a central atom?

Chem 107B: Discussion Topics – NO_x and ozone in the troposphere

1. Two options exist for significant reductions of NO_x emissions. One is to mandate reductions on emissions from approximately 30 power plants in the Midwest. The other is to mandate improved emission devices on new cars sold in the Midwest and East. These devices would add about \$750 to the cost of each new car. Each option provides about the same overall amount of reduction in NO_x emissions, and the reductions achieved by one of the options are generally regarded as representing a sufficient level of NO_x reduction under current conditions that exist in the environment. As head of the Environmental Protection Agency, which option(s) would you select. Defend your selection.

2. Should the ozone standard be tightened from its current value of 120 ppb to 80 ppb? Remember that there is general agreement that any values of ozone above the background level of 40 ppb do lead to deleterious health effects, and there is an operating assumption that the higher the value the worse, but there are no specific studies that show a discernible health advantage on going from 120 to 80 ppb.

Another way to think about this is whether we need convincing scientific data to regulate the emissions of a substance?

Chem 107B: Discussion Questions – Environmental Policy

1. Is it reasonable to enact environmental protection options that would require lifestyle changes by a significant portion of the public?
2. Current decision-making on the regulation of chemicals in the environment is done overwhelmingly on the basis of potential health effects to humans. Do you agree with such human effects being the defining criteria of whether or not a substance ought to be regulated?