Loudon Ch. 1 Review: Chemical Structure & Bonds
Jacquie Richardson, CU Boulder – Last updated 9/2/2020

Organic chemistry is focused on carbon, and is used in making pharmaceuticals and materials including polymers and liquid crystals. It's also the basis for biochemistry. It uses primarily the top three rows (a.k.a. periods) of the periodic table, plus a few elements from lower periods. The rightmost column (a.k.a. group) is the noble gases (He, Ne, etc.), and the one next to it (F, Cl, etc.) is the halogens.

	Group 1	Group 2	…	Group 13	Group 14	Group 15	Group 16	Group 17	Group 18
Period 1	H (1)								He (2)
Period 2	Li (3)	Be (4)		B (5)	C (6)	N (7)	O (8)	F (9)	Ne (10)
Period 3	Na (11)	Mg (12)		Al (13)	Si (14)	P (15)	S (16)	Cl (17)	Ar (18)
Period 4								Br (35)	
Period 5								I (53)	

The number next to each element is its atomic number, which describes the number of protons in the atom. Each atom consists of a small, heavy nucleus made up of protons (with positive charge) and neutrons (neutral, with no charge), surrounded by much lighter electrons (negative charge). Protons determine which element an atom is, electrons determine the overall charge on that atom, and neutrons don't have much effect on chemical behavior except in a few specific cases. For an atom to be electrically neutral, it must have the same number of protons and electrons. For example, a neutral fluorine atom (F) has 9 protons and 9 electrons, plus some number of neutrons.

The electrons in an atom exist in shells around the nucleus. Each shell has a maximum amount of electrons it can hold (2 for the first, 8 for subsequent shells…as far as organic chemists are concerned most of the time). The shells fill up starting closer to the nucleus and moving outwards. The electrons in filled shells are **core** electrons, and those in the unfilled outermost shell are **valence** electrons. The core electrons of each atom have the same configuration as the noble gas immediately before that atom in the table. For example, lithium (Li) has the same core electron configuration as helium (He), and chlorine (Cl) has the same core electron configuration as neon (Ne). The remaining electrons above the noble gas configuration are the valence electrons – Li has 1 valence electron, and Cl has 7.

Chemical behavior is based primarily on the behavior of valence electrons, since these are furthest from the nucleus and can interact with the "outside world" most easily. When an atom becomes a charged ion by losing or gaining electrons, it tends to do this by going to the same electron configuration as the nearest noble gas. For example, sodium (Na) has one valence electron and is closest to Ne, so it will most likely drop a single electron to become a sodium cation, Na^+. Chlorine has 7 valence electrons and will most likely pick up one more to become a chloride anion, Cl^-. (Note that because electrons have negative charge, extra electrons give something a – charge, not +. This is a very common mistake.)

Chemical Bonds
Atoms can bond together in several different ways. The two biggest subdivisions are between ionic and chemical bonds.

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Ionic bonds involve electrostatic attraction between ions, each with a complete positive or negative charge(s). The most common example is table salt, NaCl. It consists of alternating Na^+ and Cl^- ions. Each ion is surrounded by the opposite type of ion, but it has no preference for one neighboring ion over the others; there is no directionality to ionic bonds.

○ Cl^-
● Na^+
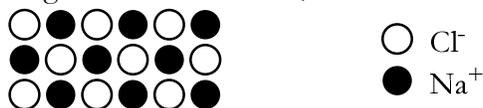
If this ionic solid were placed in something that dissolved it (for example, water in this case), each of the ions would dissociate entirely from the others and become an isolated ion.

Covalent bonds involve atoms sharing electrons, instead of losing or gaining them entirely. This is a way for multiple atoms to use the same set of electrons to get a completed shell of valence electrons – to "fill their octets" (or "duets" in the case of hydrogen, since it can only fit two electrons into its shell). The simplest example is hydrogen gas, H_2. Each hydrogen atom has a single valence electron, but pairing up with another H atom gives each one access to two shared electrons, or a filled duet. This is shown with a **Lewis dot diagram** or **Lewis structure**, where each electron is a dot. Shared electron pairs can either be shown as two dots between those atoms, or as a line linking those atoms.
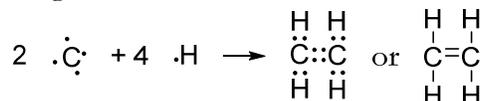
$$H\cdot + \cdot H \longrightarrow H{:}H \text{ or } H{-}H$$
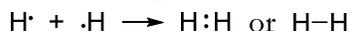
Another example is methane, or CH_4, where a central carbon atom is surrounded by four hydrogen atoms. After sharing electrons, each H atom has a filled duet and the carbon has a filled octet.

$$\cdot\ddot{C}\cdot + 4\ \cdot H \longrightarrow H{:}\ddot{\underset{\ddot{H}}{C}}{:}H \text{ or } H{-}\underset{\overset{|}{H}}{\overset{\overset{H}{|}}{C}}{-}H$$
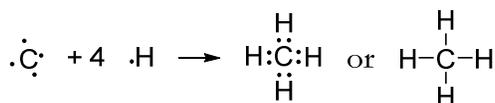
Another example is water, or H_2O. Here, oxygen already has 6 valence electrons, so it only needs to share with two hydrogen atoms for a full octet. In this case, oxygen ends up with two **lone pairs** – electrons that are not shared – as well as two shared pairs. (Later on, these lone pairs will sometimes be omitted to simplify things, although they're still implied to be there.)

$$:\!\ddot{O}\cdot + 2\ \cdot H \longrightarrow :\!\ddot{\underset{\ddot{H}}{O}}{:}H \text{ or } :\!\ddot{\underset{\overset{|}{H}}{O}}{-}H$$
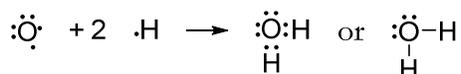
Two atoms can share more than just one pair of electrons, if that's the only way to complete their octet in a given compound. In ethene (a.k.a. ethylene), or C_2H_4, there are not enough H atoms to share electrons with each carbon. In this case, the carbon atoms share two pairs of electrons between themselves, shown as two pairs of dots between C atoms. This can also be shown as a double bond linking the carbon atoms.

$$2\ \cdot\ddot{C}\cdot + 4\ \cdot H \longrightarrow \overset{\overset{H\ H}{|\ \ |}}{\underset{\underset{H\ H}{}}{C}}{::}C \text{ or } \overset{\overset{H\ H}{|\ \ |}}{\underset{\underset{H\ H}{|\ \ |}}{C}}{=}C$$

In ethyne (a.k.a. acetylene), or C_2H_2, the carbon atoms share three pairs of electrons. This is shown as a triple bond between carbon atoms.

$$2\ \cdot\ddot{C}\cdot + 2\ \cdot H \longrightarrow H{:}C{:::}C{:}H \text{ or } H{-}C{\equiv}C{-}H$$
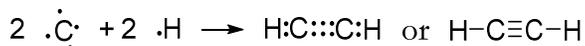
Another way to describe this is with **bond order**, the number of shared electron pairs between two atoms. The carbon atoms in ethene have a bond order of two (a double bond), while the carbon atoms in ethyne have a bond order of three (a triple bond).

It's also possible to draw Lewis structures for groups of atoms with an overall charge (polyatomic ions). If we take a boron atom and four hydrogen atoms, plus an extra electron, we get a borohydride anion - a structure with an overall negative charge. This is shown by putting square brackets around the whole thing, with a negative charge above it. Note that the charge is circled. This is common for organic chemists, since it's visually easier to keep track of charges that way and to avoid mistaking them for a bond or other line.
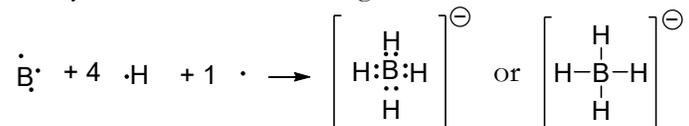
But which atom is this negative charge really on? To figure that out, we need to find the formal charge for each atom. This is equal to the number of electrons an atom needs to be neutral, minus the number it has in the structure. For the purposes of counting formal charge, each atom gets to claim all of the unshared electrons it has, plus **half** of the shared electrons. In the structure above:

- Each H atom has 0 unshared electrons plus 1 shared electron (half of the bond). Each H atom needs 1 electron to be neutral, and so has a formal charge of 1-1=0.
- The B atom has 0 unshared electrons plus 4 shared electrons (half of its bonds). The B atom needs 3 electrons to be neutral, and has a formal charge of 3-4 = -1.

This means that to draw a more specific version of the structure above, you should show the negative charge on the B atom specifically. If you do this, you should not show the charge outside square brackets. Only show one or the other.

is more accurately shown as
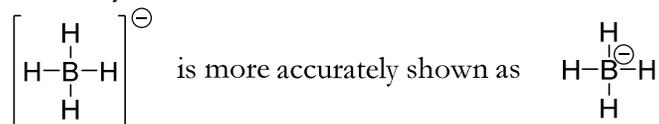
Overall, then, there are two types of ways to count electrons: octet and formal charge.

- When counting for octet, each atom counts **all** of its unshared electrons plus **all** of its shared electrons. Ideally, this number should be 2 for H, or 8 for anything else. It can be above 8 for atoms in the third period of the table and below, since these can violate the octet rule.
- When counting for formal charge, each atom counts **all** of its unshared electrons plus **half** of its shared electrons. Ideally, this number should be equal to the number of electrons on the unshared atom, so that the formal charge is zero.

Atoms are at their most stable when they have a full octet and zero charge. This means…

- Carbon generally wants four bonds and zero lone pairs
- Nitrogen generally wants three bonds and one lone pair
- Oxygen generally wants two bonds and two lone pairs
- Halogens generally want one bond and three lone pairs

Again, we will see many exceptions to these rules, but these exceptions are usually higher energy and less stable than the alternatives. One common exception: atoms in the third period of the periodic table or lower can violate the octet rule. (They do this by using d orbitals, which elements in the first & second periods don't have – see Atomic Orbitals, below.) For example, the sulfur in sulfuric acid has six bonds:

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$$\underset{O}{\overset{O}{HO-S-OH}}$$
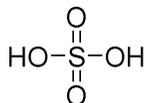
If you don't already know the connectivity of the structure, try putting the atom that needs the most bonds in the middle, or the one with the lowest electronegativity (see below).

Resonance Structures
Sometimes it's possible to draw more than one valid Lewis dot structure for a molecule. In these cases, the real molecule acts like a weighted average of all possible structures. As an example, the nitrate anion (NO_3^-) has three possible structures. These are shown with a double-headed **resonance arrow** between them.
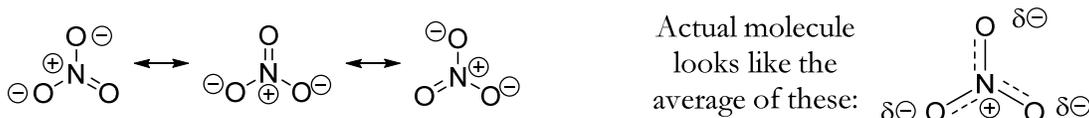
Assuming that all three states are equal in energy, which they are here, we can average together a given bond or charge across all 3 resonance forms to calculate exactly how much of a partial bond or partial charge there is. For example, if we look at the bond between N and one of the O atoms, it's a double bond in one form and a single bond in the other two forms, so on average it exists as 4/3 of a bond.

Average N-O bond order = (2 + 1 + 1) / 3 = 4/3

The average charge on an oxygen atom works the same way. Each O atom has a 2/3 charge, shown as δ⁻ on the averaged structure (δ, or "delta", just means partial).

Average charge on O = (0 + -1 + -1) / 3 = -2/3

The average charge on nitrogen is +1, so it's shown as a full positive charge on the average.

Average charge on N = (1 + 1 + 1) / 3 = 3/3 = +1

Resonance is not the same thing as equilibrium – the molecule is not moving back and forth between these three states. Instead, it exists in the averaged form all the time. The only reason we have to show different states at all is just because of the limitations of the Lewis structure system. Having resonance tends to make molecules more stable, because the charges aren't localized to a small region but can spread out over a wider area.

Polar Covalent Bonds
Just because electrons are shared between two atoms, that doesn't mean they're shared equally. If the electrons spend more time around one atom than the other, the bond is polar. How strongly an atom pulls electrons towards itself is measured by **electronegativity.** This increases up and to the right on the periodic table (ignoring noble gases since they usually don't form bonds). This means that fluorine (F) is the most electronegative (or EN for short), and the atom in the bottom left, Francium, is the least EN. As an example, Cl is more EN than H, so the electrons in a bond between H and Cl will spend more time around Cl. This can be shown in several ways – either with shading to indicate electron density, with δ (partial) charges on each atom, or with a dipole arrow. The dipole arrow always points towards the atoms with more electron density or negative charge. This is shown by making the back end of the arrow – the end over the H atom – look like a plus sign.
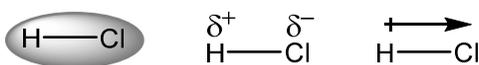
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The amount of polarization is called the dipole moment, equal to the size of the charges times the distance between them. This means that you could have the same size of dipole by having two bigger charges close together, or two small charges farther apart.

$$\overset{\delta^+}{X}\rule{2cm}{0.4pt}\overset{\delta^-}{Y} \qquad \overset{\delta^+}{X}\rule{1cm}{0.4pt}\overset{\delta^-}{Y}$$

Dipole moment is a vector, so it has both size and direction. This means that it can cancel out with other vectors. As an example, carbon dioxide, CO_2, is a linear molecule. Since its vectors are pointing in exactly opposite directions and are the same size, they cancel out perfectly. CO_2 has polar bonds, but overall it is a nonpolar molecule. In contrast, water, H_2O, is a bent molecule. Its vectors are not pointed in exactly opposite directions, so they partially cancel out but there is a net vector pointing along the middle of the molecule. H_2O has polar bonds and it is also a polar molecule.

$$O=C=O \qquad \text{Net dipole: none} \qquad\qquad \text{Net dipole: }$$
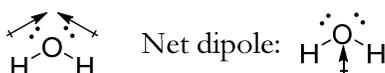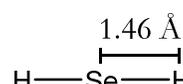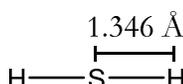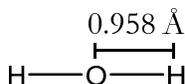
Molecular Structure

Structure is based on two things: **connectivity** (which atoms are attached to what – determined by Lewis dot structure) and **geometry** (how they are arranged in space). Geometry is defined in terms of **bond lengths**, **bond angles** and **dihedral angles**.
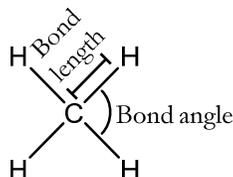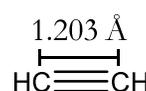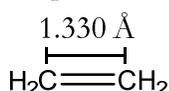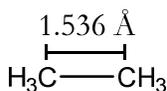

Bond lengths follow 3 main rules. All else being equal, shorter bonds are stronger bonds.

1. As you move down the periodic table, bonds get longer because the atoms are bigger.

$$\overset{0.958\,\text{Å}}{H\rule{0.5cm}{0.4pt}O\rule{0.5cm}{0.4pt}H} \qquad \overset{1.346\,\text{Å}}{H\rule{0.5cm}{0.4pt}S\rule{0.5cm}{0.4pt}H} \qquad \overset{1.46\,\text{Å}}{H\rule{0.5cm}{0.4pt}Se\rule{0.5cm}{0.4pt}H}$$

2. As the bond order increases, the bonds get shorter.

$$\overset{1.536\,\text{Å}}{H_3C\rule{0.5cm}{0.4pt}CH_3} \qquad \overset{1.330\,\text{Å}}{H_2C=CH_2} \qquad \overset{1.203\,\text{Å}}{HC\equiv CH}$$

3. As you move to the right on the periodic table, bonds get shorter because the atoms are slightly smaller. This is a much smaller effect than the other two rules.

$$\overset{1.091\,\text{Å}}{H_3C\rule{0.5cm}{0.4pt}H} \qquad \overset{1.008\,\text{Å}}{H_2N\rule{0.5cm}{0.4pt}H} \qquad \overset{0.958\,\text{Å}}{HO\rule{0.5cm}{0.4pt}H}$$
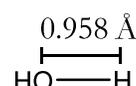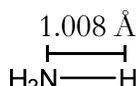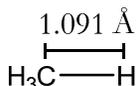
Bond angles are determined by Valence Shell Electron Pair Repulsion theory, or VSEPR (pronounced "vesper"). This is based on the idea that groups (lone pairs, atoms, or groups of atoms) are arranged around a central atom in a way that spreads them out as much as possible. The exact shape depends on how many groups are attached to the central atom.
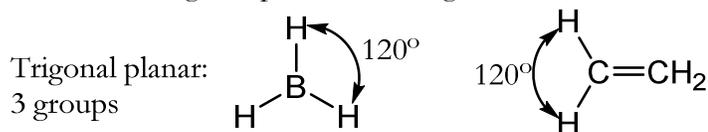
- 2 groups on central atom: linear, with angles of 180°.
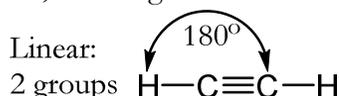
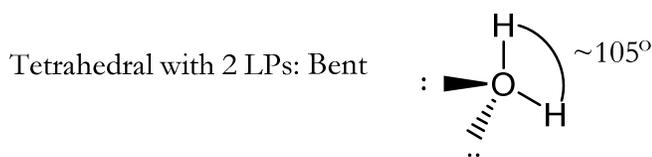$$\text{Linear:} \qquad \overset{180^\circ}{}$$
$$\text{2 groups} \quad H-C\equiv C-H$$

- 3 groups on central atom: trigonal planar, with angles of 120°.

Trigonal planar:
3 groups

- 4 groups on central atom: tetrahedral, with angles of 109.5°. Since this is the only one of the three that can't be laid out flat in a plane, this is the first time we'll see wedge (or bold) and dashed bonds. This is a way to show that bonds are coming out of the plane of the paper towards you, or going into the plane away from you.

Tetrahedral:
4 groups

Bold bonds are coming out towards you

Dashed bonds are going away from you
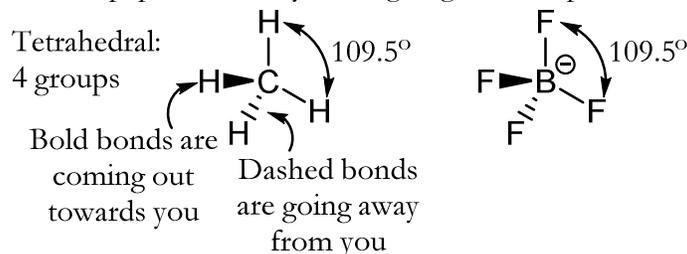
If one or more of these groups is a lone pair, we can't "see" them. In these cases, the electronic geometry (arrangement of all groups including lone pairs) is still following the rules above, but the molecular geometry (arrangement of all groups **except** lone pairs) is different. Also, since a lone pair takes up slightly more than its fair share of space, it squeezes together the other groups so they're a degree or two away from the usual bond angles.

Trigonal planar with 1 LP: Bent

Tetrahedral with 1 LP: Trigonal pyramidal

Tetrahedral with 2 LPs: Bent
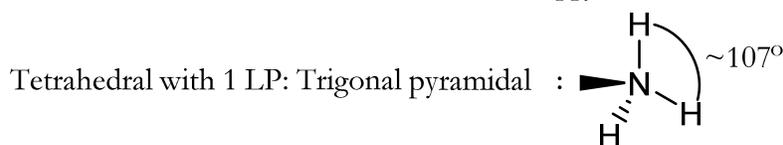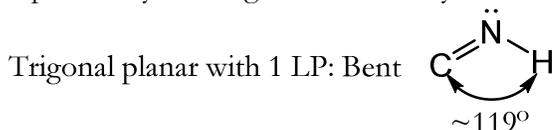
Dihedral angles, or torsional angles, describe rotation around the central bond in a four-atom chain. For example, hydrogen peroxide (H_2O_2) is shown below with two different dihedral angles. Even though the bond angles don't change (they're still about 105°), the dihedral angle changes as the molecule rotates around its central bond. The "dihedral angle" is how close the two end atoms appear to be from each other, when viewed from the end.

180° dihedral

0° dihedral

Atomic Orbitals
Even though we show electrons as dots with defined locations, that's not strictly accurate – they have wavelike character too. The exact position can't be specified, only the likelihood that they'll be in a particular area. We can describe this area using atomic orbitals (AOs).

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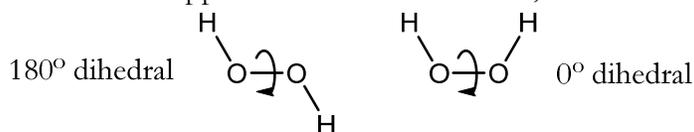(A lot of these rules may seem arbitrary. They actually will make complete sense once you take physical chemistry, since they're based on interactions of the three-dimensional integrals used to generate the wavefunctions. For now, just go with it.)

These are calculated using wavefunctions based on 3 quantum numbers:

1. Principal quantum number (n): Tells you the size and energy of the orbital. Possible values are counting numbers - 1, 2, 3, 4, etc. Higher numbers are larger and higher energy because they're farther from the nucleus.
2. Angular momentum quantum number (ℓ, or cursive l): Tells you the shape of the orbital. Possible values are 0 to (n-1). So if n is 3, then ℓ can be 0, 1, or 2. If ℓ is 0, the orbital is an s-orbital or sphere. If ℓ is 1, the orbital is a p-orbital or dumbbell. If ℓ is 2, the orbital is a d-orbital – these can be a couple of different shapes
3. Magnetic quantum number (m_ℓ): Tells you the orientation of the orbital. Possible values are $-\ell$ to $+\ell$. This just defines how many different possible orbitals there are at that energy level.

For example, if you have an orbital with n=2 and ℓ=0, it would have to have m_ℓ = 0. This would be a 2s orbital, a spherical shell around the nucleus. If you have an orbital with n=2 and ℓ=1, it could have m_ℓ = -1, 0, or 1. Each of these would be separate orbitals, named $2p_x$, $2p_y$, and $2p_z$, all perpendicular to each other. Which one is which doesn't matter in the absence of external factors.

2s orbital   2p orbital

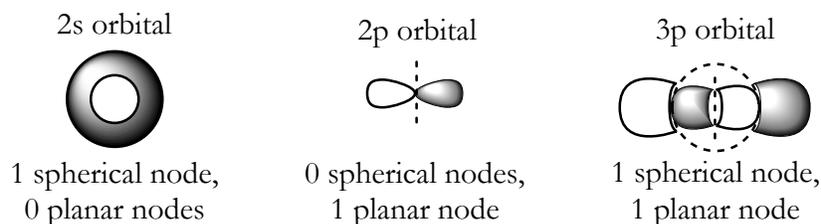$m_\ell = 0$ $m_\ell = -1$ $m_\ell = 0$ $m_\ell = 1$
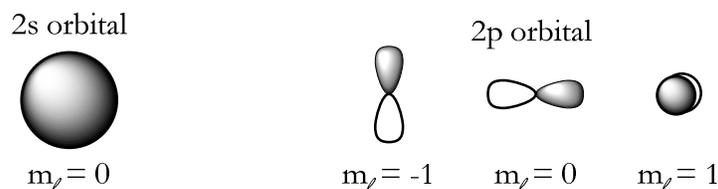
These can be thought of as standing waves of a probability function, which means they have crests (positive values) and troughs (negative values). This doesn't mean that the charge on the electron can be positive or negative, only the function that describes its location. These two phases – positive and negative – are usually shown as red and blue parts of an orbital, or dark and light like the two parts of the p orbitals above.

Node (zero amplitude)   Positive amplitude

Negative amplitude
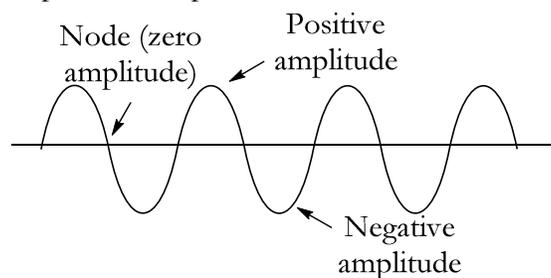
Where the wave goes from positive to negative or vice versa, it passes through a point where it has a value of zero. This is a node – an area where the electron has zero probability of being located. (The probability than an electron will be found in a particular place is actually the square of the wavefunction value, since probabilities can't be negative.) There are two types of nodes: spherical and planar. The number of nodes an orbital has is based on its quantum numbers. Each orbital has (n-1) total nodes, of which ℓ nodes are planar. This implies that each orbital has (n-1-ℓ) spherical nodes. In 3-dimensional orbital shapes, the nodes are any boundaries between light and dark orbital lobes.

2s orbital

2p orbital

3p orbital

1 spherical node,
0 planar nodes

0 spherical nodes,
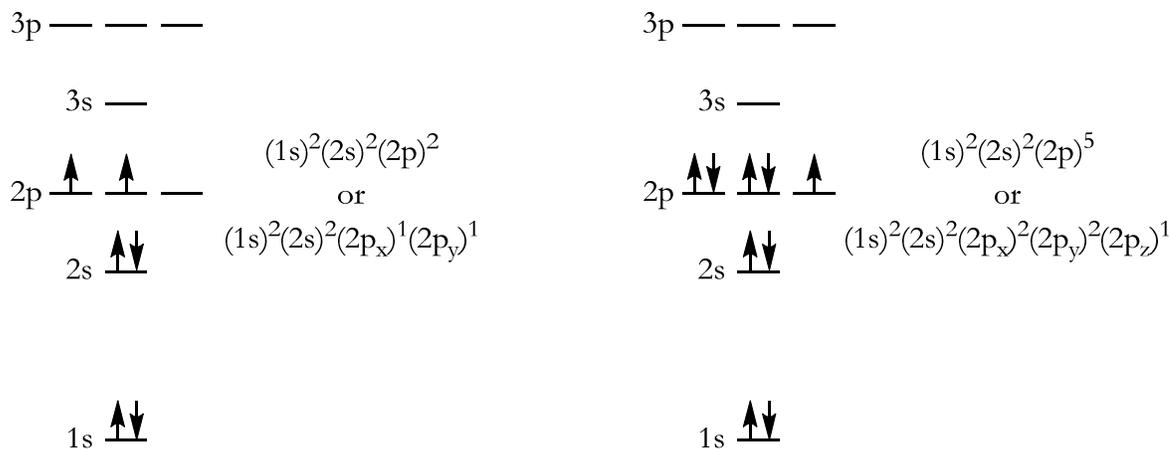1 planar node

1 spherical node,
1 planar node

Once these orbital shapes are figured out, the next step is filling them with electrons. This brings up a fourth quantum number, spin (m_s). For an electron, this can be either $+\frac{1}{2}$ ("up") or $-\frac{1}{2}$ ("down"). The **Pauli Exclusion Principle** says that no two electrons in an atom can have all four quantum numbers the same. This means only two electrons can fit into each orbital where n, ℓ, and m_ℓ are already set. To figure out which orbitals to put the electrons into for a given atom, follow the **Aufbau Principle**: start at the lowest energy orbitals (lowest n values) and put two electrons in each orbital, one up and one down. If there are multiple orbitals at the same energy, follow **Hund's Rule**: put one electron into each of them first, all with the same spin, then go back and give them each a second one if you still have enough electrons.

Some examples of how to fill orbitals are shown below for carbon and fluorine. For both atoms, the valence electrons are the ones with the highest n number. In both of these cases, the 2s and 2p orbitals hold valence electrons. The electron configuration is written next to each orbital diagram – the number of electrons in each orbital is indicated by a superscript. Different orientations of p orbitals can be grouped together, or listed separately.

Carbon (6 electrons):

Fluorine (9 electrons):

3p — — —

3p — — —

3s —

3s —

2p ↑ ↑ —

$(1s)^2(2s)^2(2p)^2$
or
$(1s)^2(2s)^2(2p_x)^1(2p_y)^1$

2p ↑↓ ↑↓ ↑

$(1s)^2(2s)^2(2p)^5$
or
$(1s)^2(2s)^2(2p_x)^2(2p_y)^2(2p_z)^1$

2s ↑↓

2s ↑↓

1s ↑↓

1s ↑↓

Hybrid Orbitals

The tetrahedral geometry we saw for most octet-rule-following atoms doesn't match up with the perpendicular shape of the p orbitals. As it turns out, when there are other atoms around, most atoms will **hybridize** some of their s and p orbitals together. This costs energy at first, but allows the atom to form stronger bonds, ultimately making up for it. Hybrid orbitals are named after the AOs that make them up. For example, a hybrid of one s orbital and three p orbitals will create four new sp^3 orbitals (the total number is conserved). These happen to point towards the four corners of a tetrahedron.
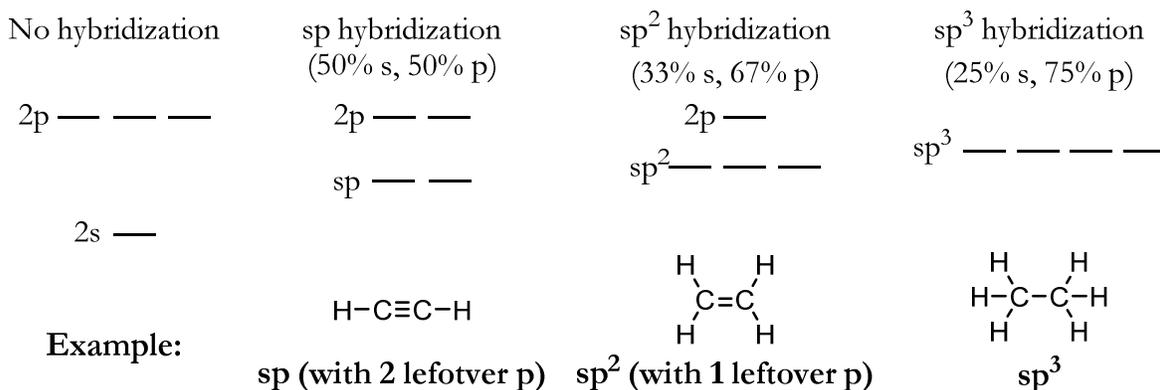
Loudon Ch. 1 Review: Chemical Structure & Bonds

Jacquie Richardson, CU Boulder – Last updated 9/2/2020

 Tetrahedral sp^3 atom
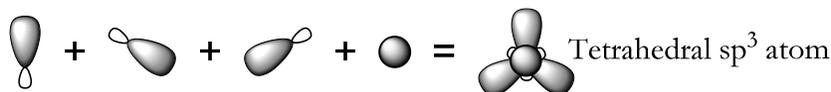
The total number of hybrid orbitals is equal to the number of groups on an atom according to VSEPR, so an atom with 4 groups would be sp^3-hybridized (tetrahedral), an atom with 3 groups would be sp^2-hybridized (trigonal planar), and an atom with 2 groups would be sp-hybridized (linear). Any leftover, unhybridized p orbitals stick out perpendicular to the hybridized orbitals. They can be used to form double and triple bonds, or left empty depending on circumstances.

Each hybrid orbital is the average of its components, so for example an sp^3 hybrid has 25% s and 75% p character. The more s character an orbital has, the closer it will be to the nucleus, since s orbitals are closer to the nucleus than p. This means that single bonds to sp^3 carbons are slightly longer than single bonds to sp^2, since sp^3 carbons make bonds with more p character. The energy of hybrid orbitals is close to the average energy of the AOs that were hybridized together – an energy diagram is shown below. Note that any p orbitals that don't get hybridized (leftover p orbitals) stay at the same level.

No hybridization	sp hybridization (50% s, 50% p)	sp^2 hybridization (33% s, 67% p)	sp^3 hybridization (25% s, 75% p)

2p ⎯ ⎯ ⎯   2p ⎯ ⎯   2p ⎯ sp^3 ⎯ ⎯ ⎯ ⎯

sp ⎯ ⎯ sp^2 ⎯ ⎯ ⎯

2s ⎯

Example:

H−C≡C−H
sp (with 2 lefotver p)

H₂C=CH₂ (C=C with H, H / H, H)
sp^2 (with 1 leftover p)

H−C−C−H (with H's)
sp^3

Molecular Orbitals

Once we start looking at molecules, the electrons belong to more than just one atom. We need a way to describe orbitals for combinations of atoms. Molecular Orbital or **MO Theory** can do this, by the following process:

1. The individual AOS are shown on the left and right sides of the MO diagram.
2. Combine AOs to get MOs:
    a. Number of orbitals is conserved (2 AOs give 2 MOs). Show which AOs made which MOs with dotted lines.
    b. Head-on overlap between orbitals creates σ orbitals; side-on overlap creates π orbitals (we'll see these in Ch. 4). **The first bond between any two atoms is σ and any additional bonds are π. Side-on overlap is usually less significant and raises/lowers the energy of new MOs by less.**
    c. Orbitals can combine with constructive or destructive interference – in other words, dark can match with dark, or dark can mismatch with light. Each of these options gives the two possible new MOs from a pair of AOs:
        i. Constructive interference creates orbitals with no new nodes. These "bonding MOs" are lower in energy, and marked with σ or π.
        ii. Destructive interference creates orbitals with a new node. These "antibonding MOs" are higher in energy, and marked with σ* or π*.
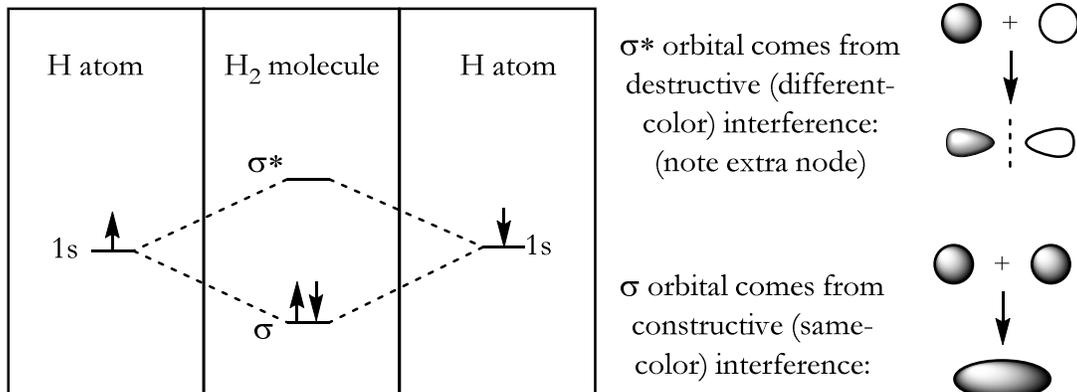
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        iii. Unused AOs will carry over into the middle, unchanged in energy. These "nonbonding MOs" are the same energy as their parent AOs, and are normally used for lone pairs or empty orbitals on atoms.

3. Fill MOs by Aufbau principle/Hund's rule.
4. The bond order between two atoms is given by (number of electrons in bonding orbitals - number of electrons in antibonding orbitals)/2.

Let's use H_2 as an example. The H atoms appear on the sides of the MO diagram, while the new H_2 molecule appears in the center. The two 1s orbitals from the H atoms combine to form two new orbitals: σ, the bonding orbital, and σ*, the antibonding orbital. Since σ* is based on destructive interference, it has one more node, which makes it higher in energy. Once the levels are constructed, we can start filling in electrons. Each H atom arrives with one electron, so they are combined to put two electrons in the H_2 molecule. These both fill into the σ orbital, which gives a bond order of 1.

σ* orbital comes from destructive (different-color) interference: (note extra node)

σ orbital comes from constructive (same-color) interference:

Bond order = (2-0)/2 = 1

The reason MO diagrams is so useful is because they can also cover cases that don't work in Lewis dot structures. For example, the H_2^- ion has three electrons (one from each H atom and one extra for the negative charge). The shapes and names of the orbitals stay the same, but we have one extra electron to place, which drops the bond order to ½.
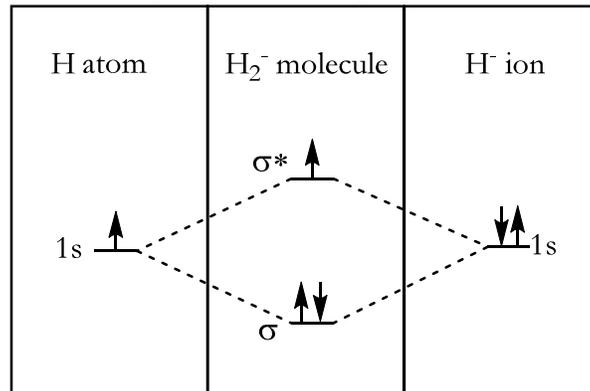
Bond order = (2-1)/2 = 1/2

As an example of π bonds, we can use alkenes. These are any molecule with a C=C double bond, so the carbon atoms have 1 σ bond and 1 π bond. The carbon atoms are sp^2-hybridized: one of the 2p orbitals stays unhybridized, but the other two 2p orbitals mix with

the 2s to form sp^2 hybrids. VSEPR predicts that the σ bonds formed with these sp^2 orbitals are trigonal planar, with the leftover p orbital sticking out above and below the plane.

Leftover p orbitals extend above and below plane

To form a π bond, the two leftover p orbitals come together above and below the plane. Just like before when we looked at σ orbitals, we can bring these p orbitals together with same-color overlap (to get constructive interference) or opposite-color overlap (to get destructive interference). These two options will generate our two new MOs. At the same time, these atoms still have the head-on overlap of their sp^2 orbitals, which generates the σ orbital (lower than π) and σ* orbital (higher than π*). Note that only one sp^2 orbital is used for each carbon, since the other ones are used to form C-H bonds that are not shown here.

sp^2 C atom	C=C bond	sp^2 C atom
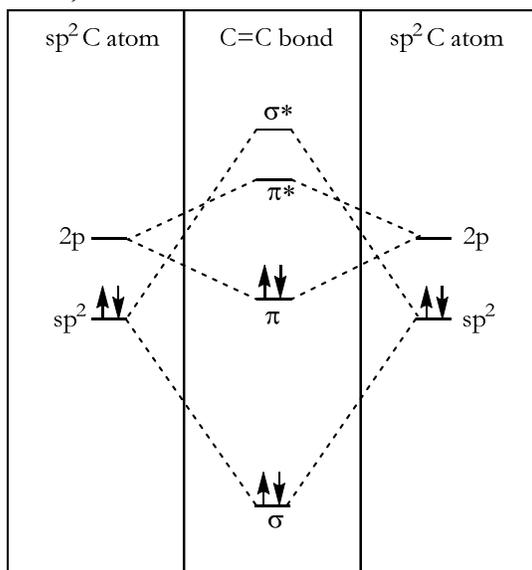
σ* orbital from destructive head-on overlap of sp^2 orbitals

π* orbital comes from destructive side-on overlap of p orbitals

π orbital comes from constructive side-on overlap of p orbitals

σ orbital comes from constructive head-on overlap of sp^2 orbitals

Bond order = (4-0)/2 = 2