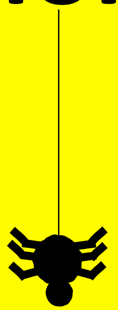
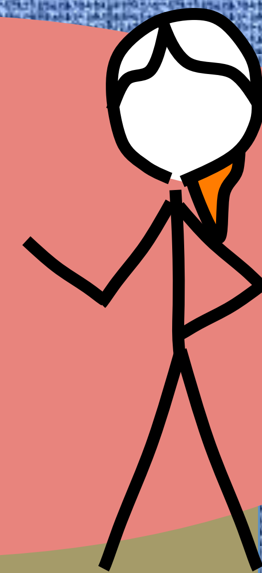
Experiment 9
29 October 2019
Molecular Shapes



This presentation is a self-guided lesson on Lewis dot structures and molecular shape.

Objective: To learn how to predict molecular shape and associated properties.

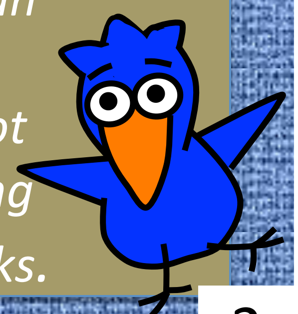
Today we will learn to correctly sketch good Lewis dot structures...



... and use them to predict molecular shape and other properties.

Overview:

1. Drawing Lewis dot structures
2. From Lewis structures to shape
3. Molecular polarity, hybridization, resonance, and paramagnetism
4. Expanded octets
5. Summary and what we do today

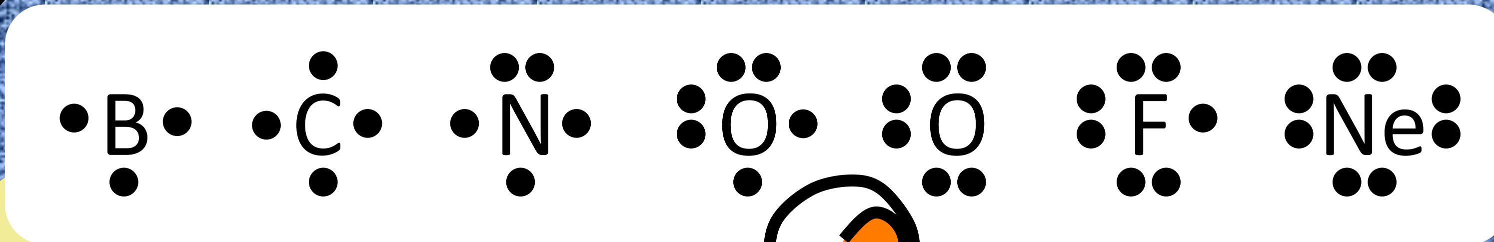


No need to write an introduction this week. We will not be writing anything in our lab notebooks.

1. Drawing Lewis dot structures

We start with the Lewis dot structure of each atom. These are their n = 2 valence electrons (2s + 2p) shown as pairs of dots.

Notice oxygen comes in two styles. Weird. More on this later…

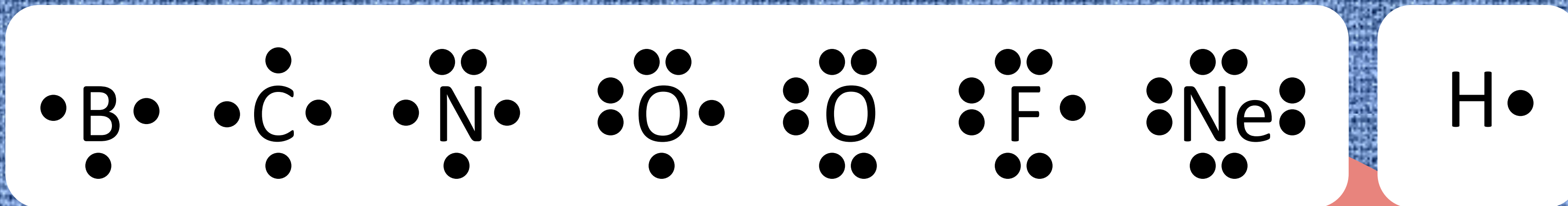


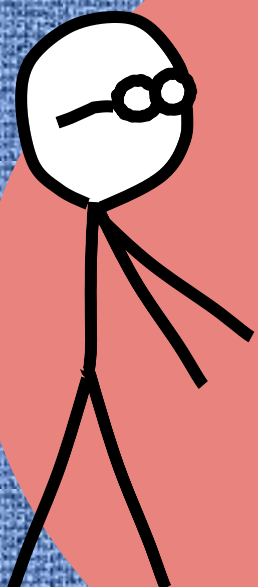
Here are the 2nd row main group elements, boron, carbon, nitrogen, oxygen, fluorine and neon, each with their Lewis dots.

Lewis's objective is for each atom to have eight electrons (four pairs) – an octet. As you can see, neon already has eight and is good to go.

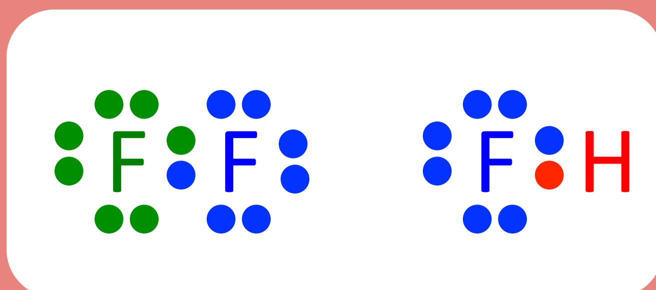
Hydrogen and helium want only two electrons.

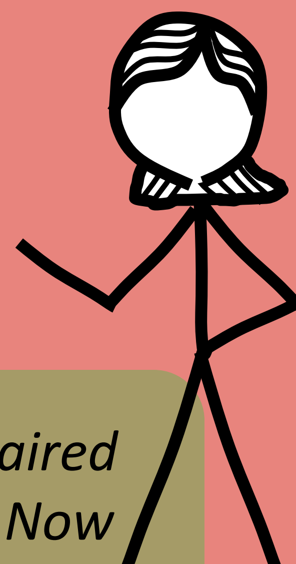
1. Drawing Lewis dot structures



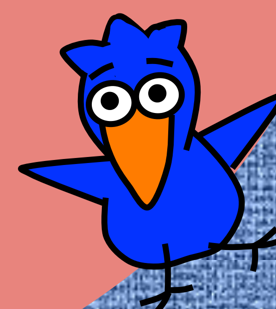


Neon may have an octet and is "happy," but fluorine has only seven valence electrons and wants one more to fulfill its octet.



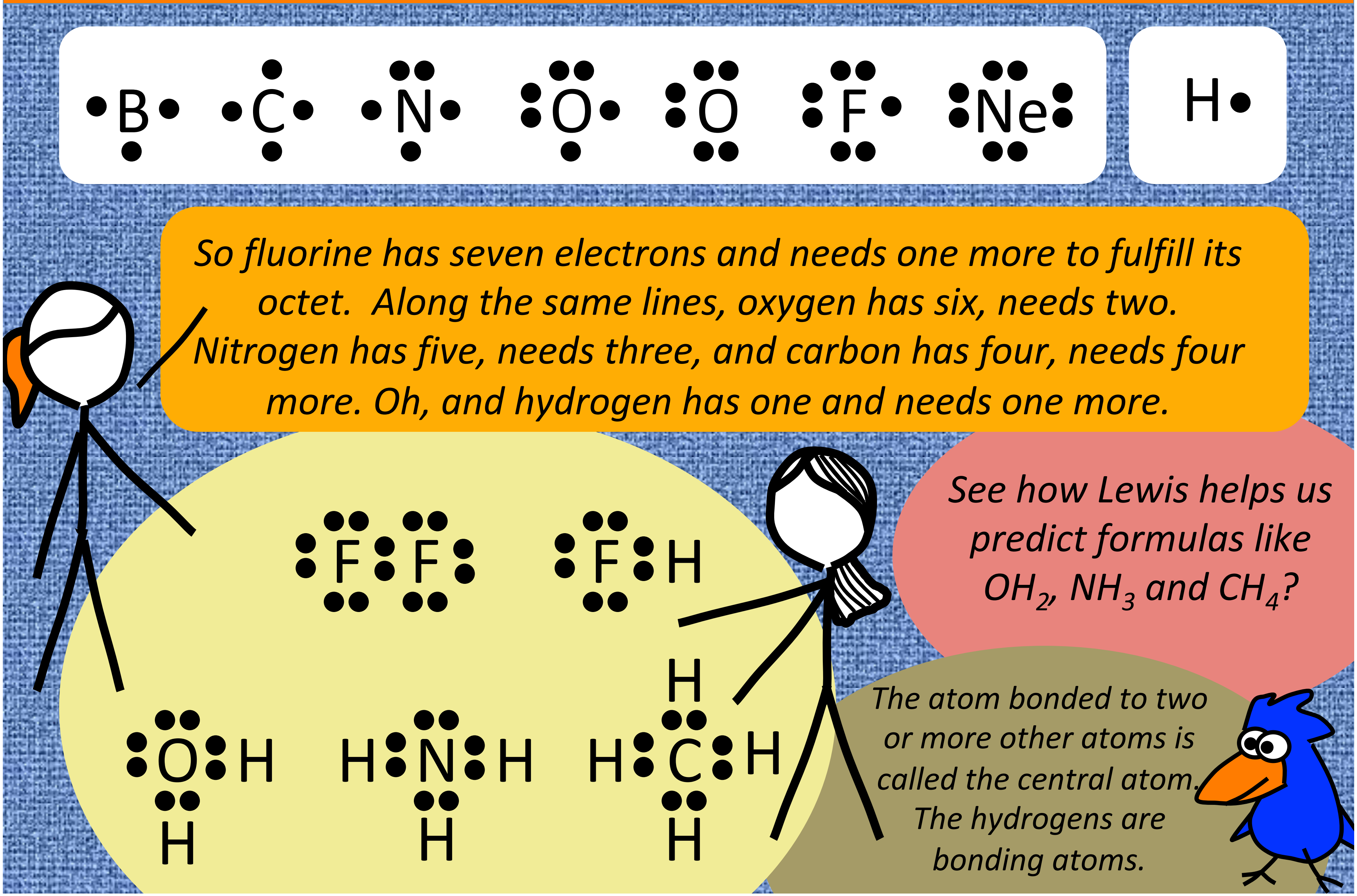


An electron shared bond is a covalent bond.

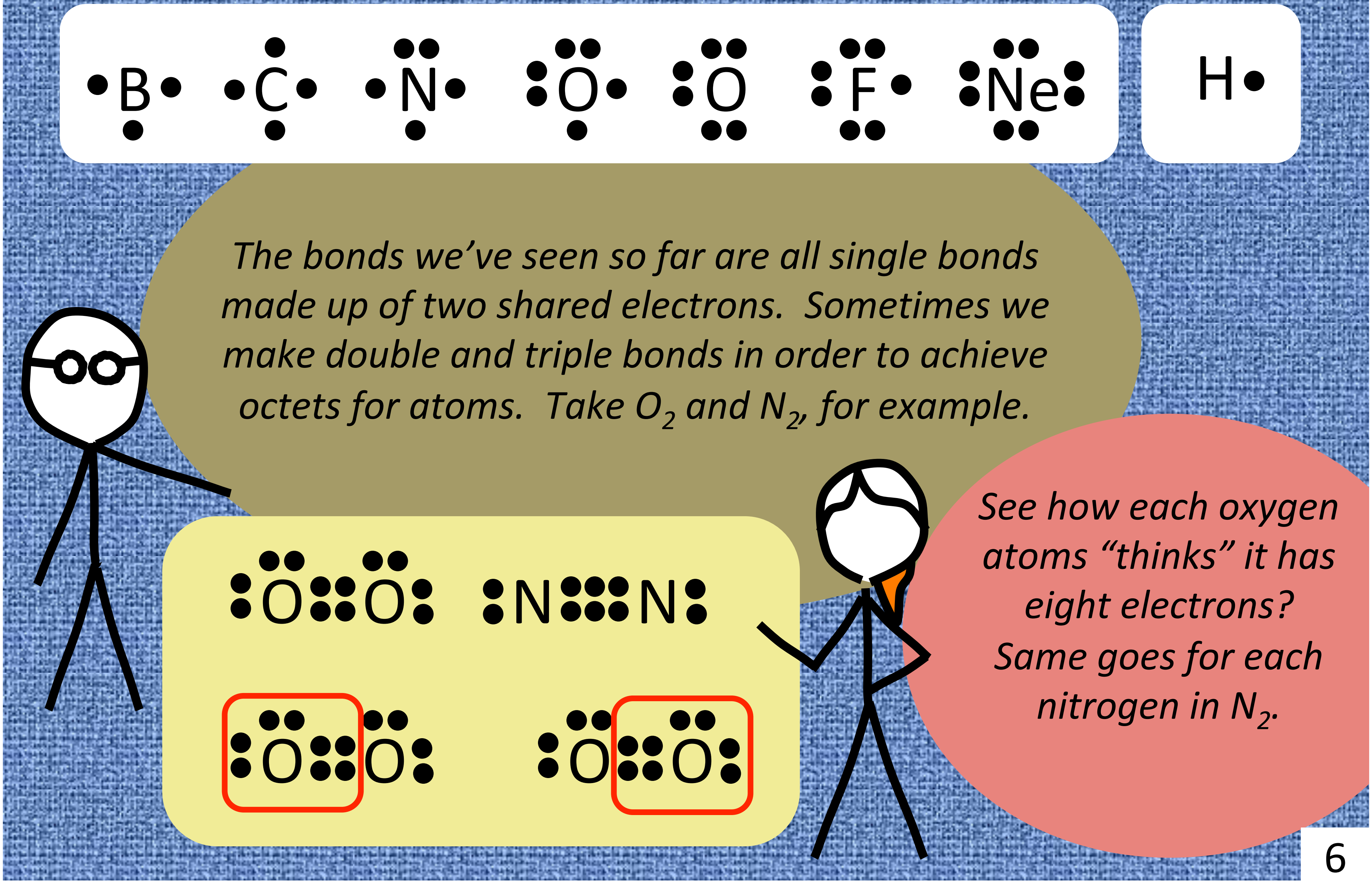


One way to accomplish this is to share its unpaired electron with another fluorine or a hydrogen. Now each has an octet or duplet in the case of hydrogen.

1. Drawing Lewis dot structures



1. Drawing Lewis dot structures



1. Drawing Lewis dot structures

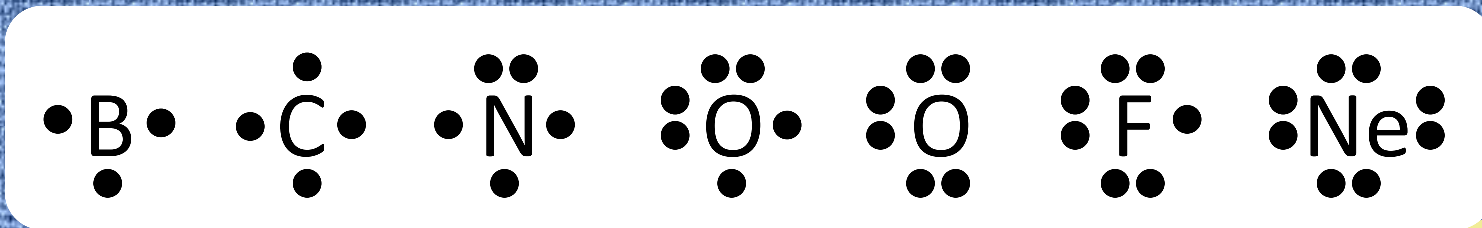
B C N O O F Ne

H

Ooo! I finally have a slide to myself! Here is a cute trick. The atoms that we've seen are representative of the other atoms below them on the periodic table. They have the same Lewis dot structures.

B	C	N	O	O	F	Ne
Al	Si	P	S	S	Cl	Ar
Ga	Ge	As	Se	Se	Br	Kr

1. Drawing Lewis dot structures

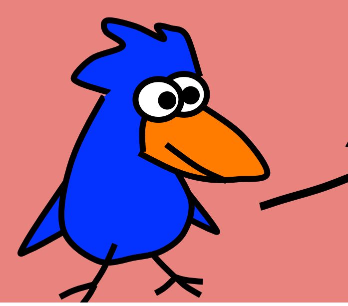


We are now ready for more challenging molecules and polyatomic ions with covalent bonds. For this we need a simple procedure we can follow.

Step 1. Sketch out the atoms involved like above – or refer to the drawing above.

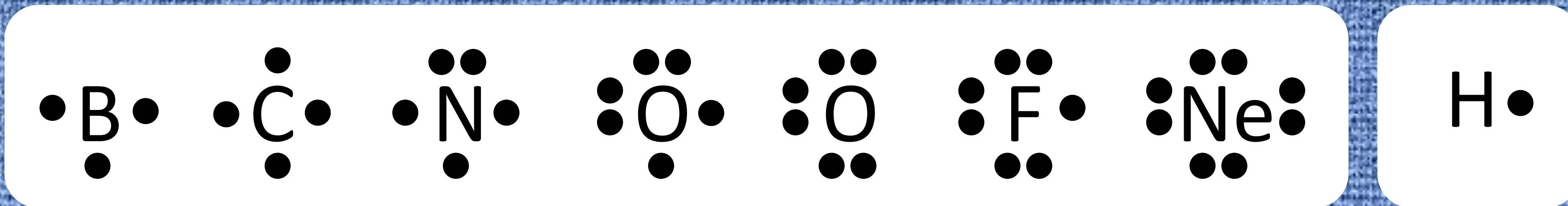
Step 2. Adjust the central atom for the charge on the ion if it is an ion. Make them look like their neighbors. For example, N^+ will look like carbon. N^- would look like oxygen.

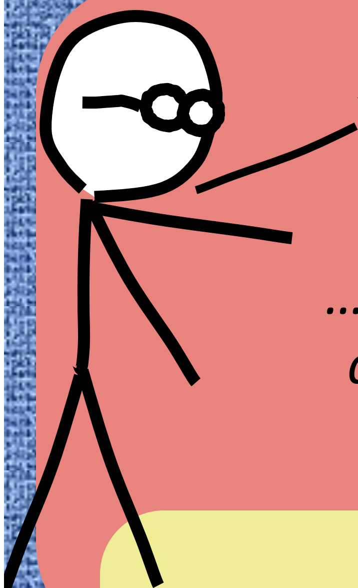
Our first example will be the ammonium ion, $\boldsymbol{NH_4^+}$.



And now for Step 3…

1. Drawing Lewis dot structures



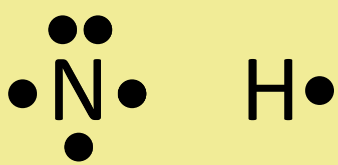


And Step 3 is…

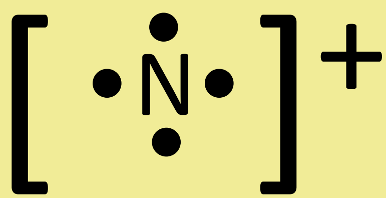
Step 1. Sketch atoms.

Step 2. Adjust central atom for charge.

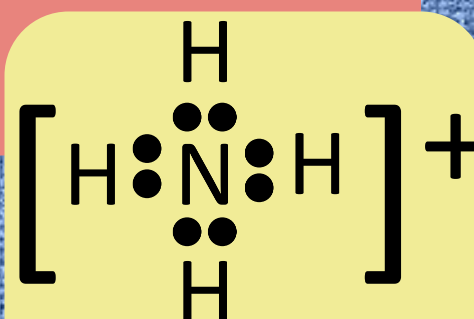
… Add the bonding atoms ***one at a time*** *to the central atom. Remember that the goal is to make everyone have an octet (or for H, duplet).*



Step 1.

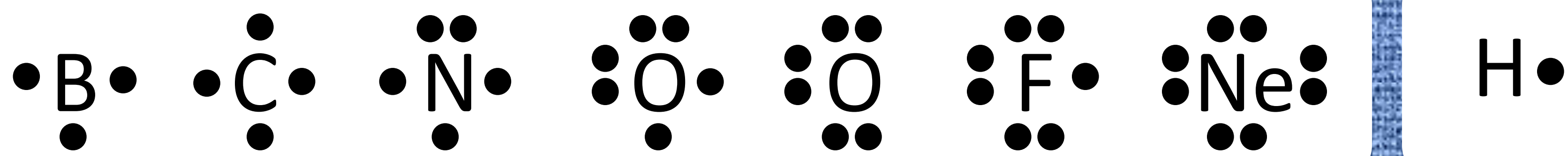


Step 2.



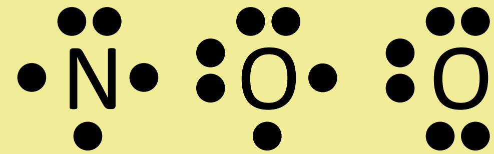
Step 3.

1. Drawing Lewis dot structures

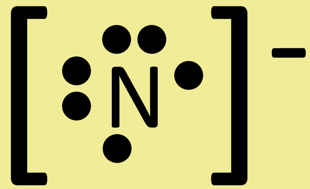


Our next example will be nitrite ion, $\mathbf{NO_2^-}$.

Step 1. Sketch atoms.



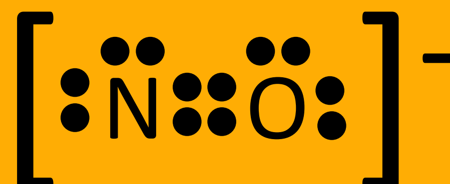
Step 1.



Step 2.

Step 2. Adjust central atom for charge.

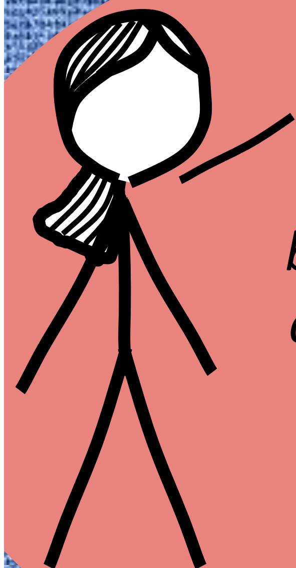
*Step 3. Add the bonding atoms **one at a time** to the central atom. If oxygen is a bonding atom, start with it because it needs to make a double bond in order to make an octet.*



Step 3.

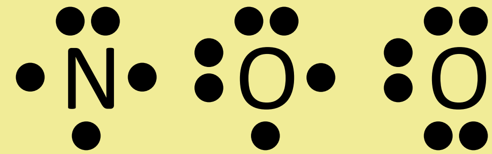
That's just the first oxygen!

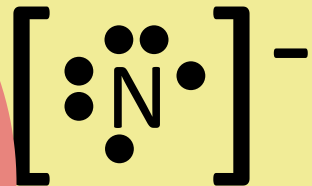
1. Drawing Lewis dot structures



*So after adding the first oxygen, both atoms have an octet! Nitrite (**NO_2^-**) needs another oxygen… so...*

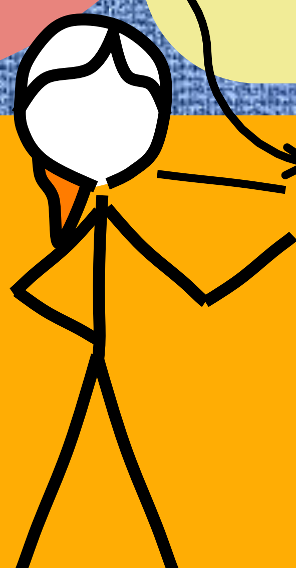
Step 1. Sketch atoms.

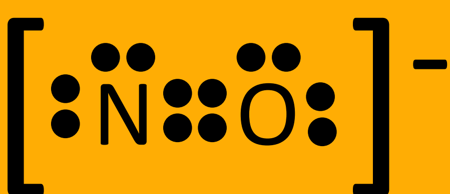




Step 2. Adjust central atom for charge.

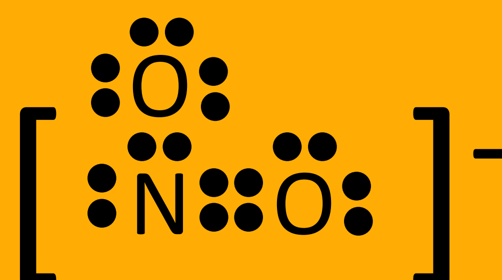
Step 3. Add the bonding atoms **one at a time** to the central atom. If oxygen is a bonding atom, start with it because it needs to make a double bond in order to make an octet.



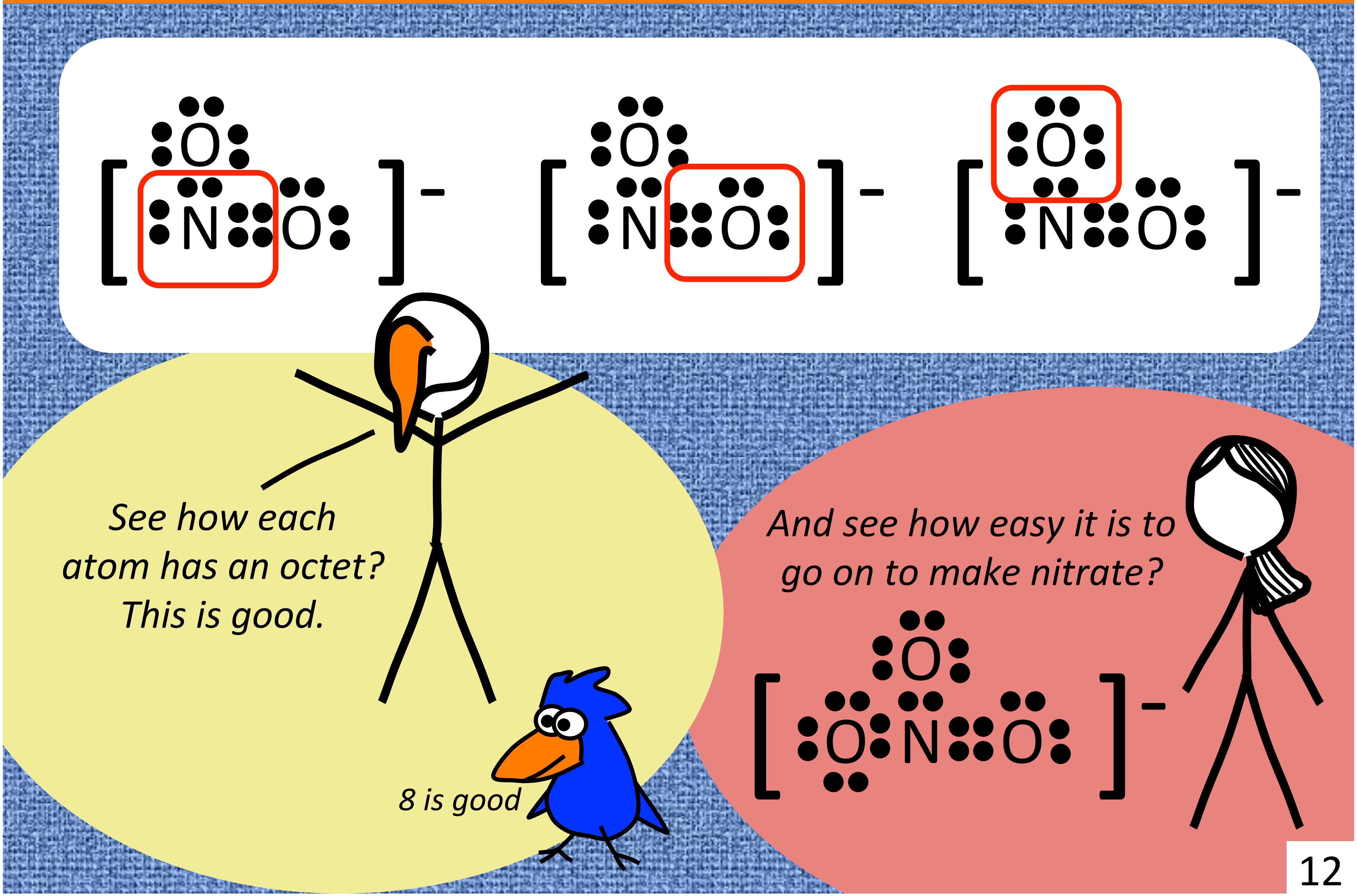


Step 3 – first atom added.

… we add the second oxygen using the other style oxygen so all atoms have an octet.

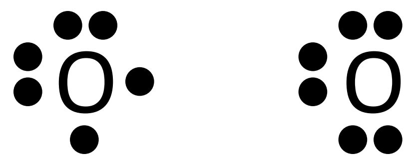


1. Drawing Lewis dot structures



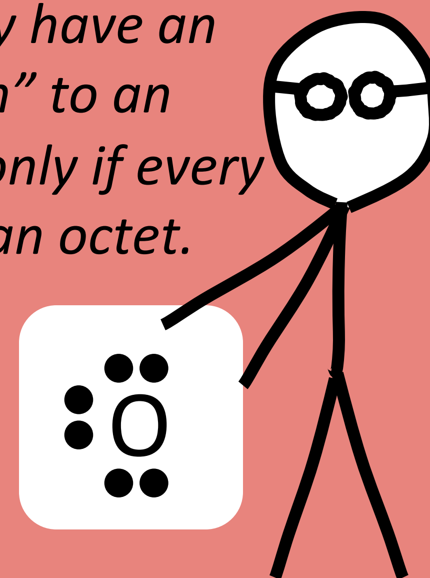
1. Drawing Lewis dot structures

Normal and snap-on oxygen

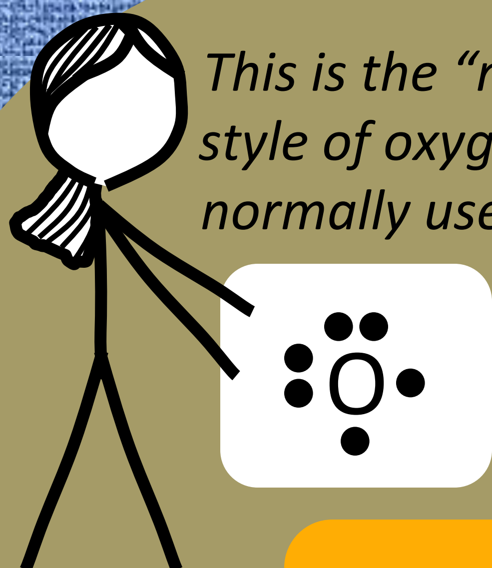


This is the oxygen used when the other atoms already have an octet. It "snaps on" to an electron pair. Use it only if every atom already has an octet.

Ooo! Snap-on oxygen!



This is the "normal" style of oxygen. We normally use it first.

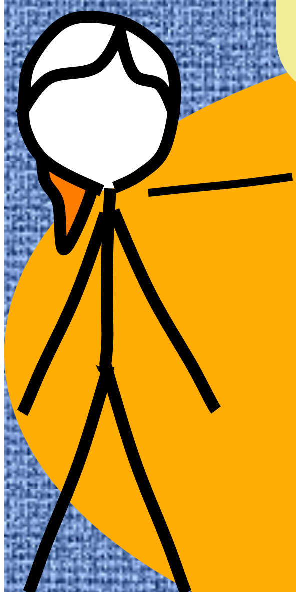


1. Sketch atoms.
2. Adjust central atom for charge.
3. Add bonding atoms one at a time starting with O.

1. Drawing Lewis dot structures

The three steps for making good Lewis dot structures

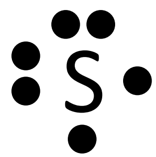
1. Sketch atoms.
2. Adjust central atom for charge.
3. Add bonding atoms one at a time starting with O.



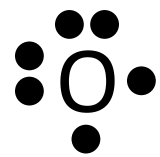
Let's try a few more examples. How about sulfur dioxide, SO_2 and sulfur trioxide, SO_3.

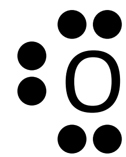
Here is Step 1. Step 2 is not needed this time.

Sulfur

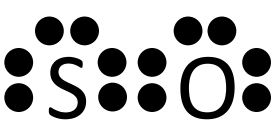


Normal and snap-on oxygen

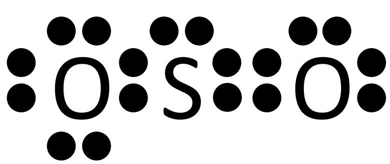




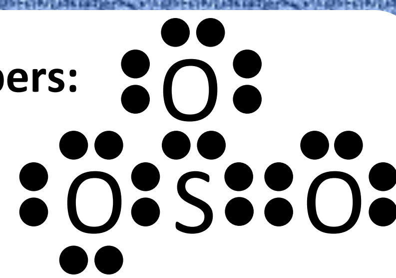
Sulfur + normal oxygen



… and a snap-on O:



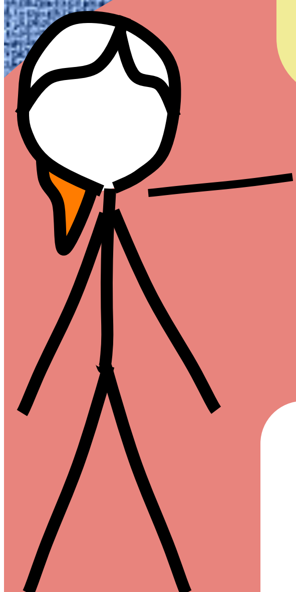
And 2 snappers:



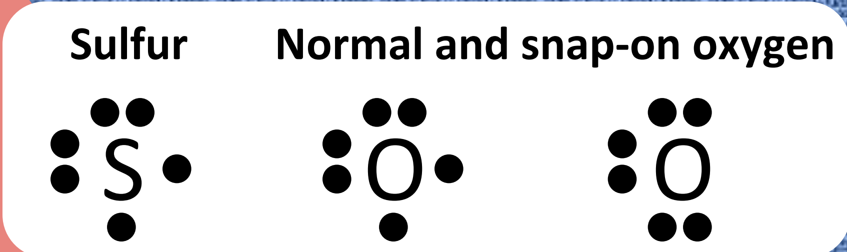
1. Drawing Lewis dot structures

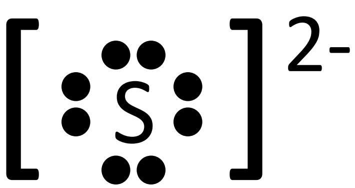
The three steps for making good Lewis dot structures

1. Sketch atoms.
2. Adjust central atom for charge.
3. Add bonding atoms one at a time starting with O.

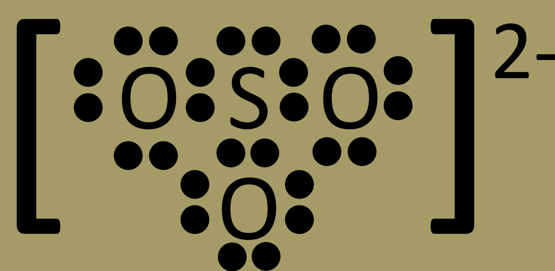


How about sulfite, SO_3^{2-} and sulfate, SO_4^{2-}? Here are Steps 1 and 2

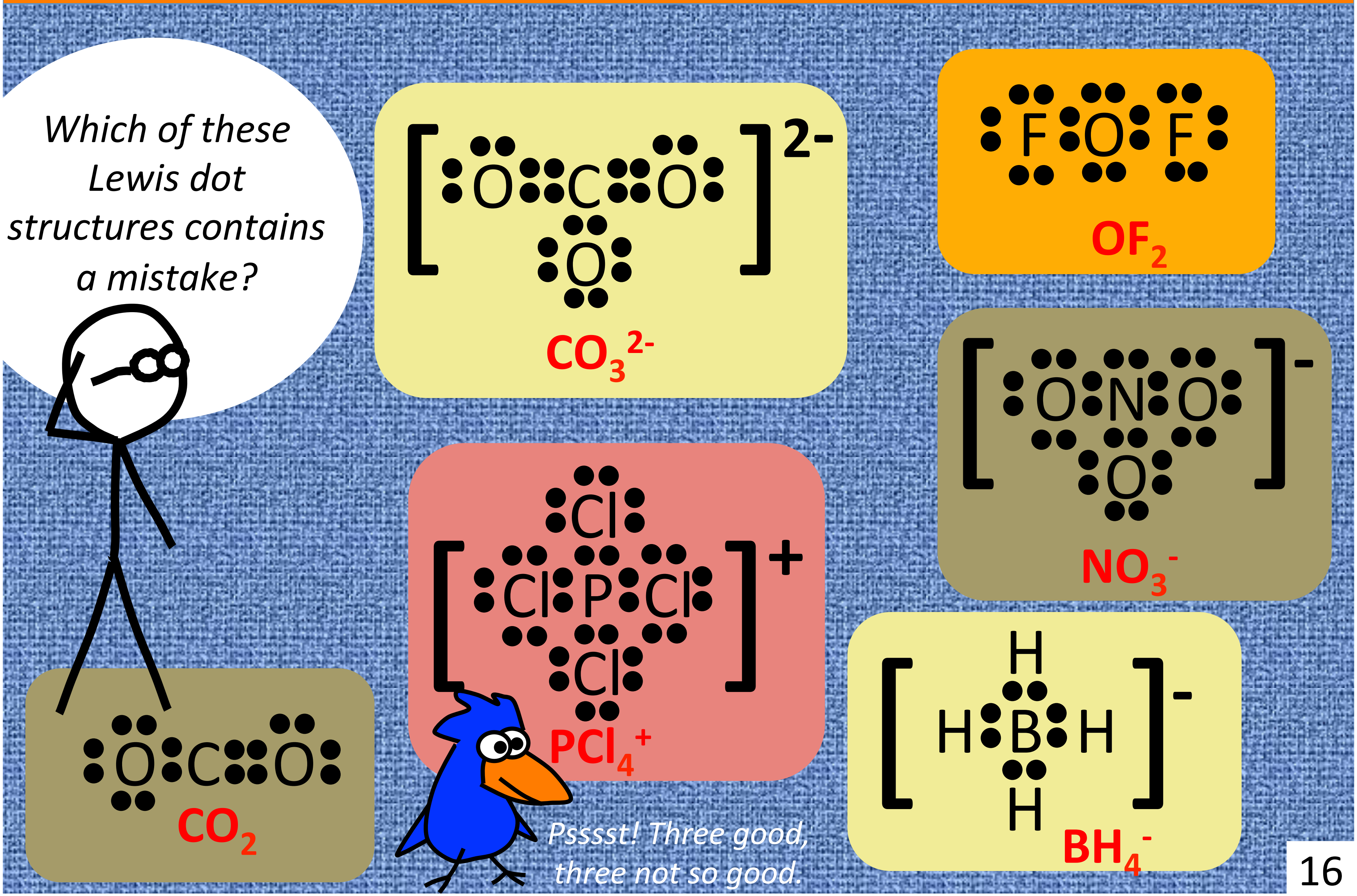




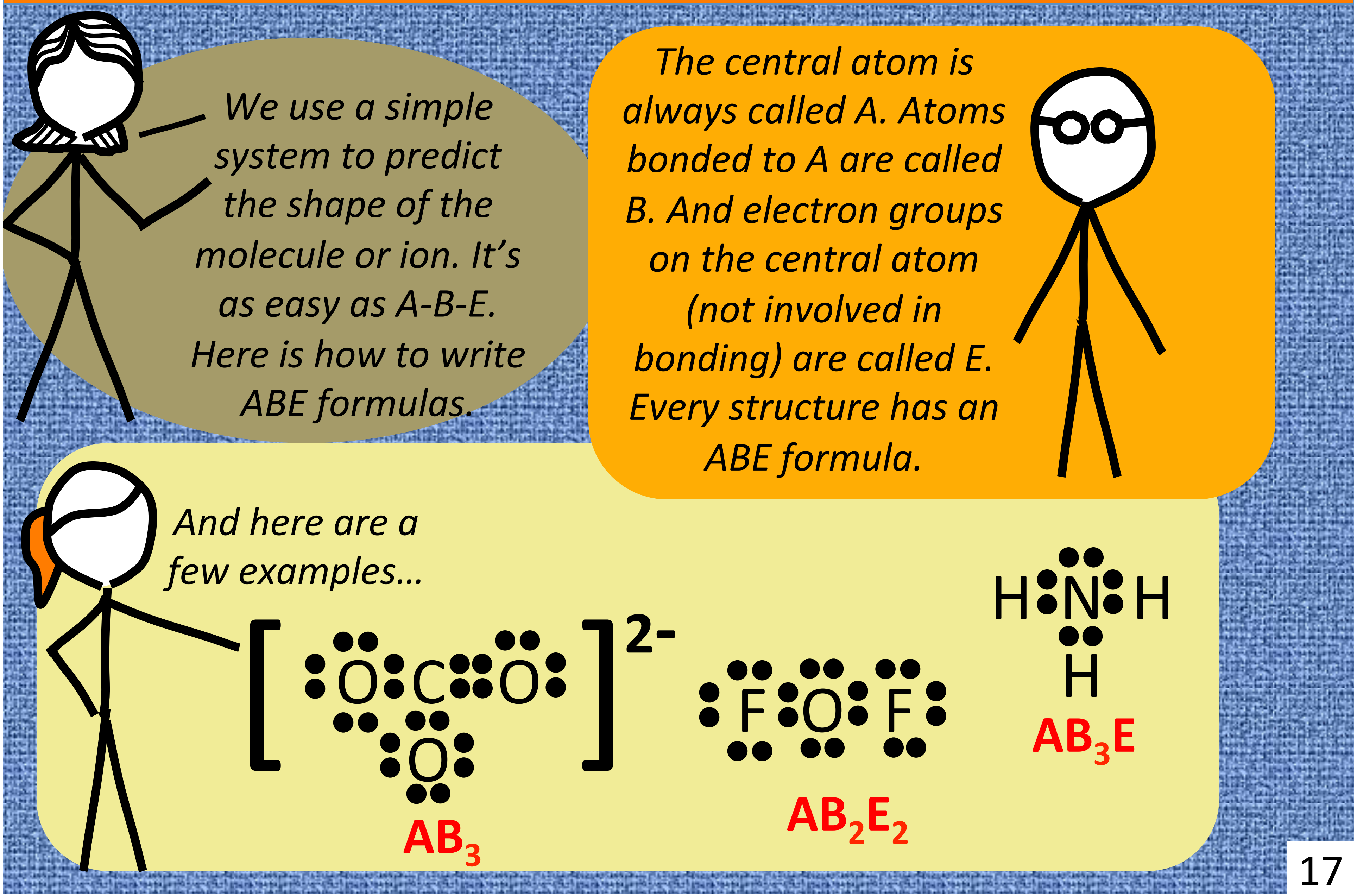
After Step 2, we see that sulfur already has an octet. We go straight to snap-ons! Here is sulfite:



1. Drawing Lewis dot structures

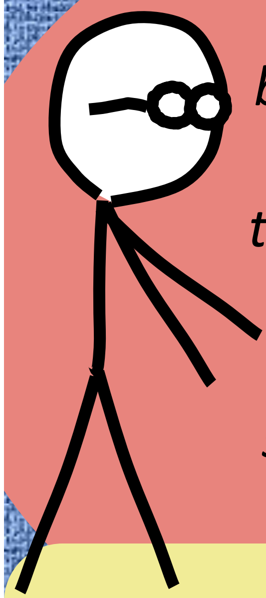


2. From Lewis structures to shape



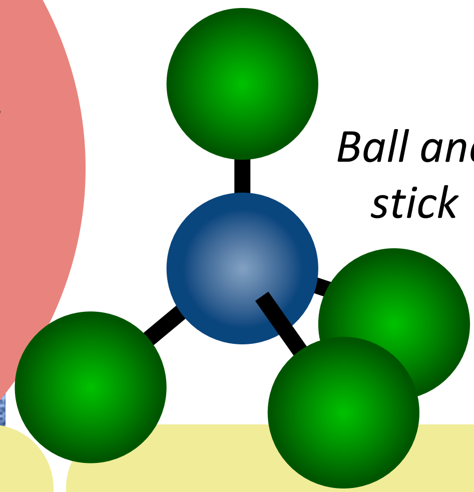
2. From Lewis structures to shape: 4 Groups

Lewis structure → ABE Formula → Shape

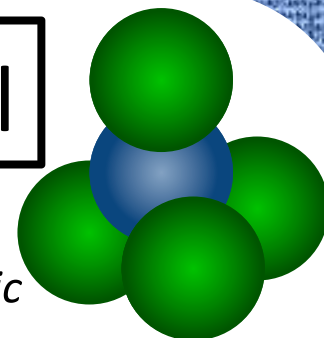


The examples shown below are all examples of AB_4. Every AB_4 has the tetrahedral structure in 3-dimensions. Angles are all 109°. And here are some ways to sketch AB_4 structures.

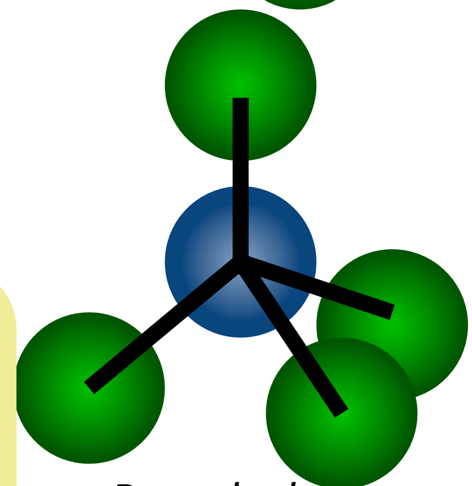
AB_4 tetrahedral



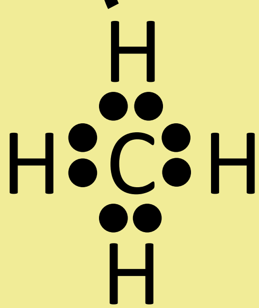
Ball and stick

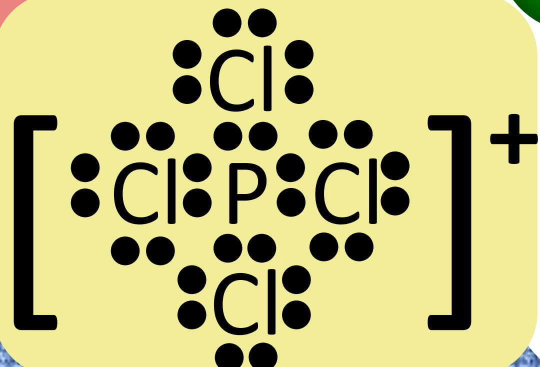


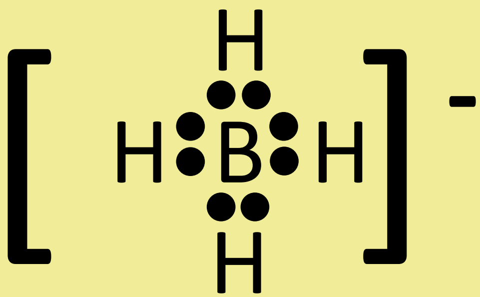
More realistic



Reveals the tetrahedral angle of 109°





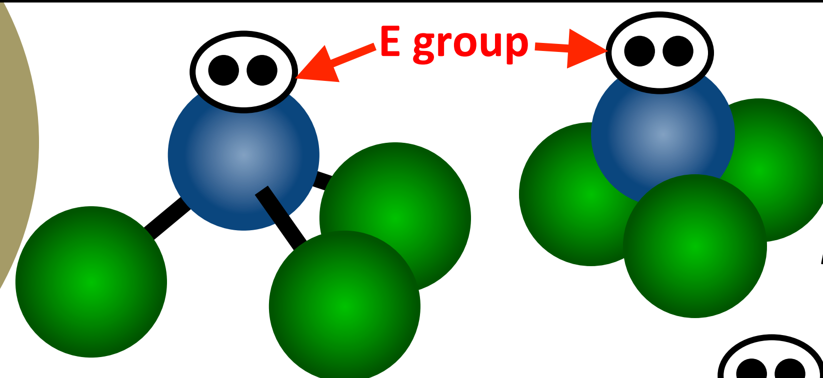


2. From Lewis structures to shape: 4 Groups

Lewis structure → ABE Formula → Shape

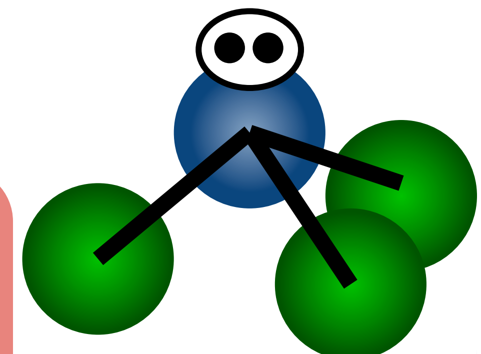
These examples are all AB_3E. Every AB_3E has four groups total just like AB_4, so the angles are close to 109^o – a little less because the E group pushes the B groups together a bit.

AB_3E trigonal pyramid

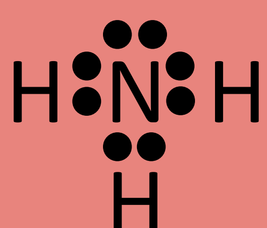


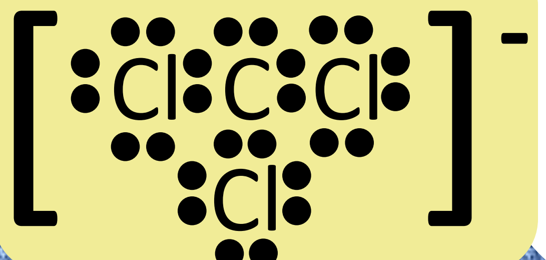
Ball and stick

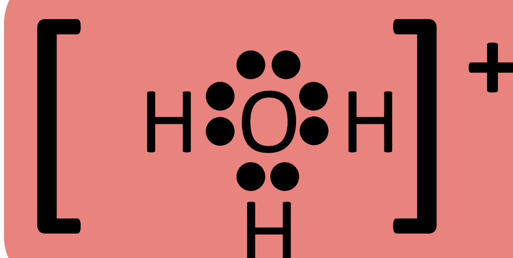
More realistic



Reveals the near tetrahedral angle

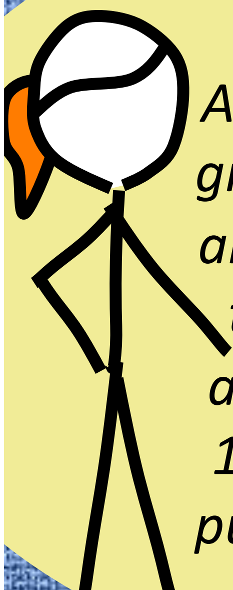






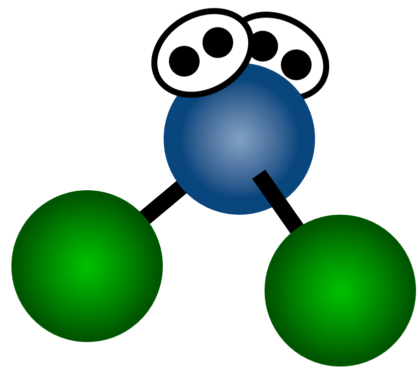
2. From Lewis structures to shape: 4 Groups

Lewis structure → ABE Formula → Shape

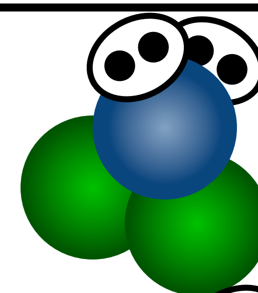


These examples are all AB_2E_2. Every AB_2E_2 has four groups total – two B groups and two E groups. Like with the trigonal pyramid, the angles are a little less than 109^o because the E groups push the B groups together.

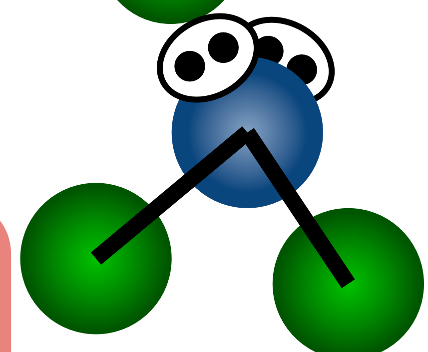
AB_2E_2 bent (based on tetrahedron)



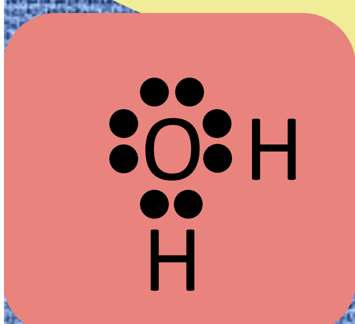
Ball and stick

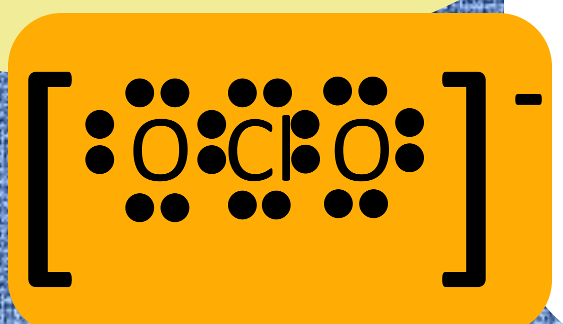


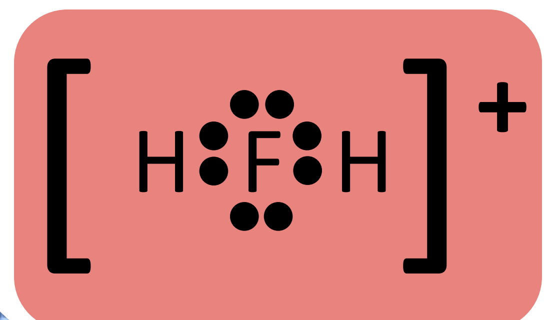
More realistic



Reveals the near tetrahedral angle of ~<109^o

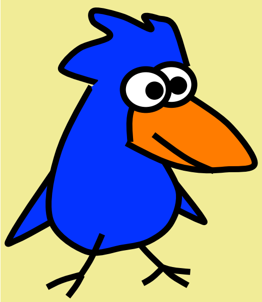






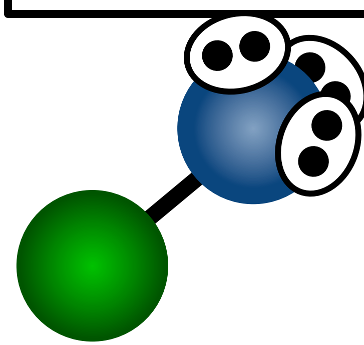
2. From Lewis structures to shape: 4 Groups

Lewis structure → ABE Formula → Shape

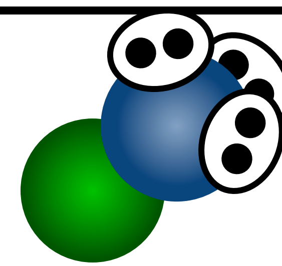


The last 4-group combinations are ABE_3 and AE_4. ABE_3 has only two atoms, so the thing is linear. AE_4 is just something with an octet, such as Cl^- or Ar…

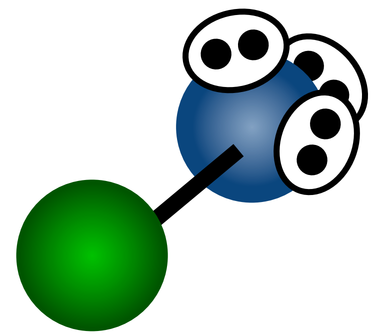
ABE_3 linear



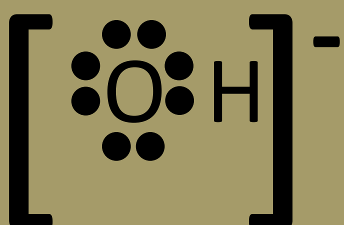
Ball and stick



More realistic



We need three atoms to have an angle

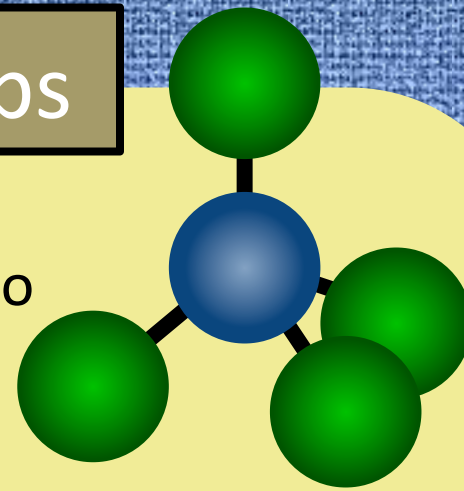


2. From Lewis structures to shape: 4 Groups

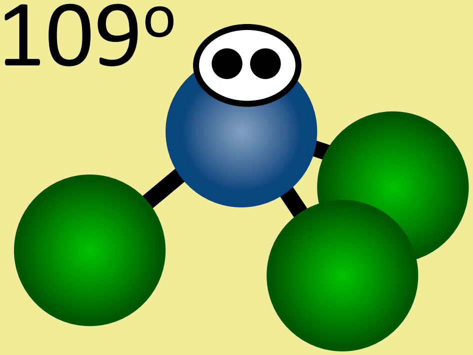
Summary of 4 Groups

This sums up all possible Lewis dot structures with 4 groups

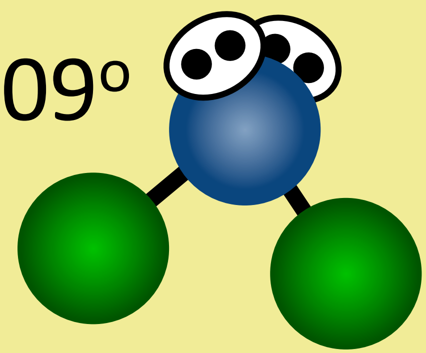
AB_4 Tetrahedron 109^o



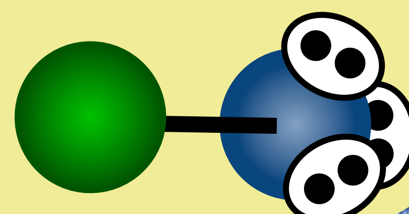
AB_3E Trigonal bipyramid $<109^o$



AB_2E_2 Bent $<109^o$



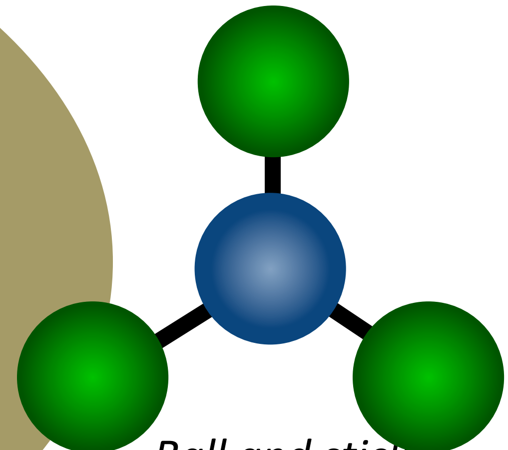
ABE_3 Linear



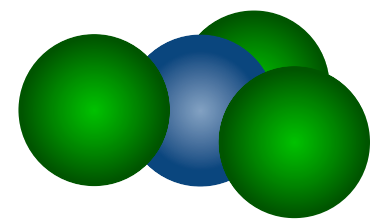
2. From Lewis structures to shape: 3 Groups

Now that we've studied ABE structures with 4 groups, let's look at those with three groups. The possibilities are AB_3, AB_2E, and ABE_2. All three are based on the trigonal plane with angles of close to 120°.

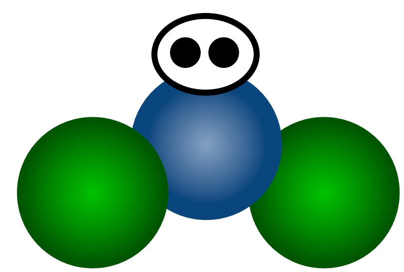
AB_3 (trigonal plane) and AB_2E (bent) (based on 120° trig. plane)



Ball and stick
Trigonal plane, 120°

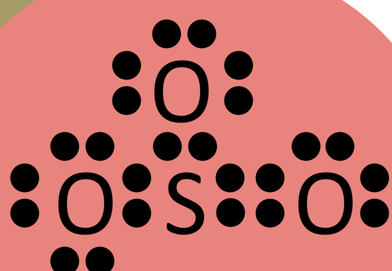


Most realistic (side view)

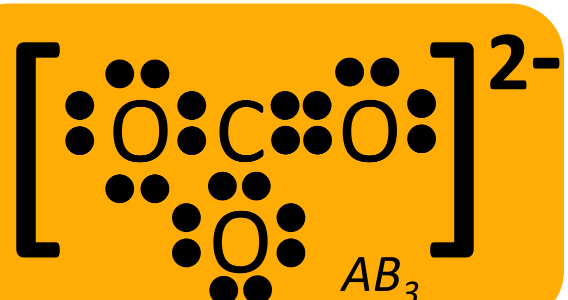


Top view of AB_2E with ~< 120° angle (bent)

AB_2E



AB_3

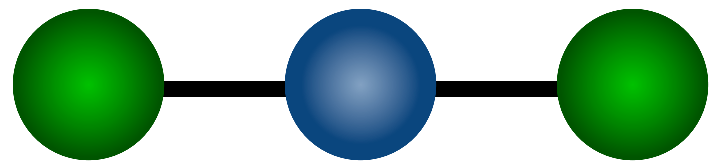


AB_3

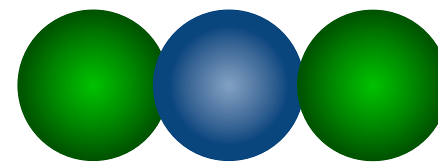
2. From Lewis structures to shape: 2 Groups

Finally, we have the situation with only two groups around the central atom – either AB_2 or ABE. The angle in AB_2 is 180°. ABE is also linear, but with two atoms we don't talk about angles.

AB_2 and ABE (linear)



Ball and stick
linear, 180°



Most realistic
(side view)

$:\ddot{O}::C::\ddot{O}:$

AB_2

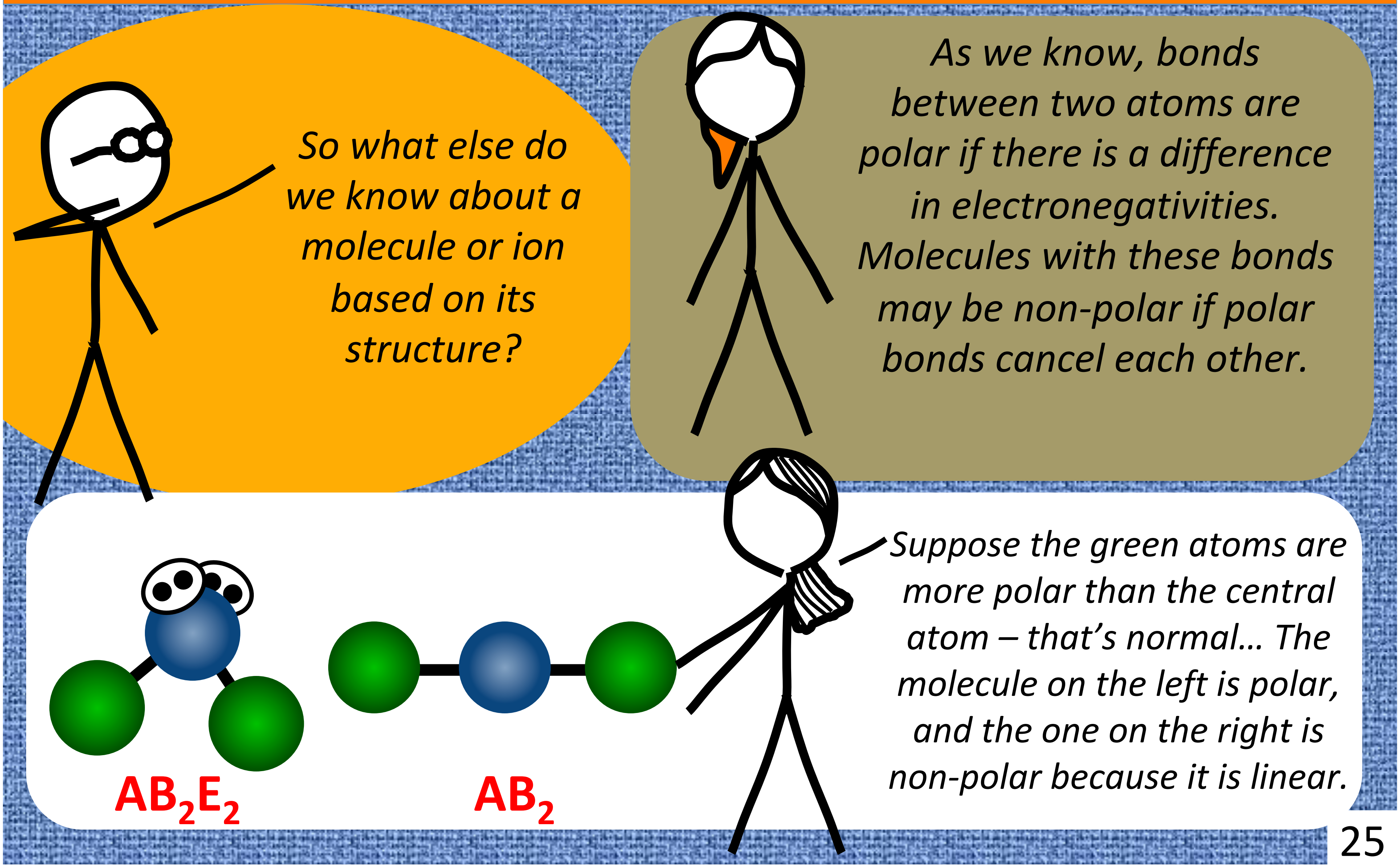
$H:C:::N:$

AB_2 *ABE*

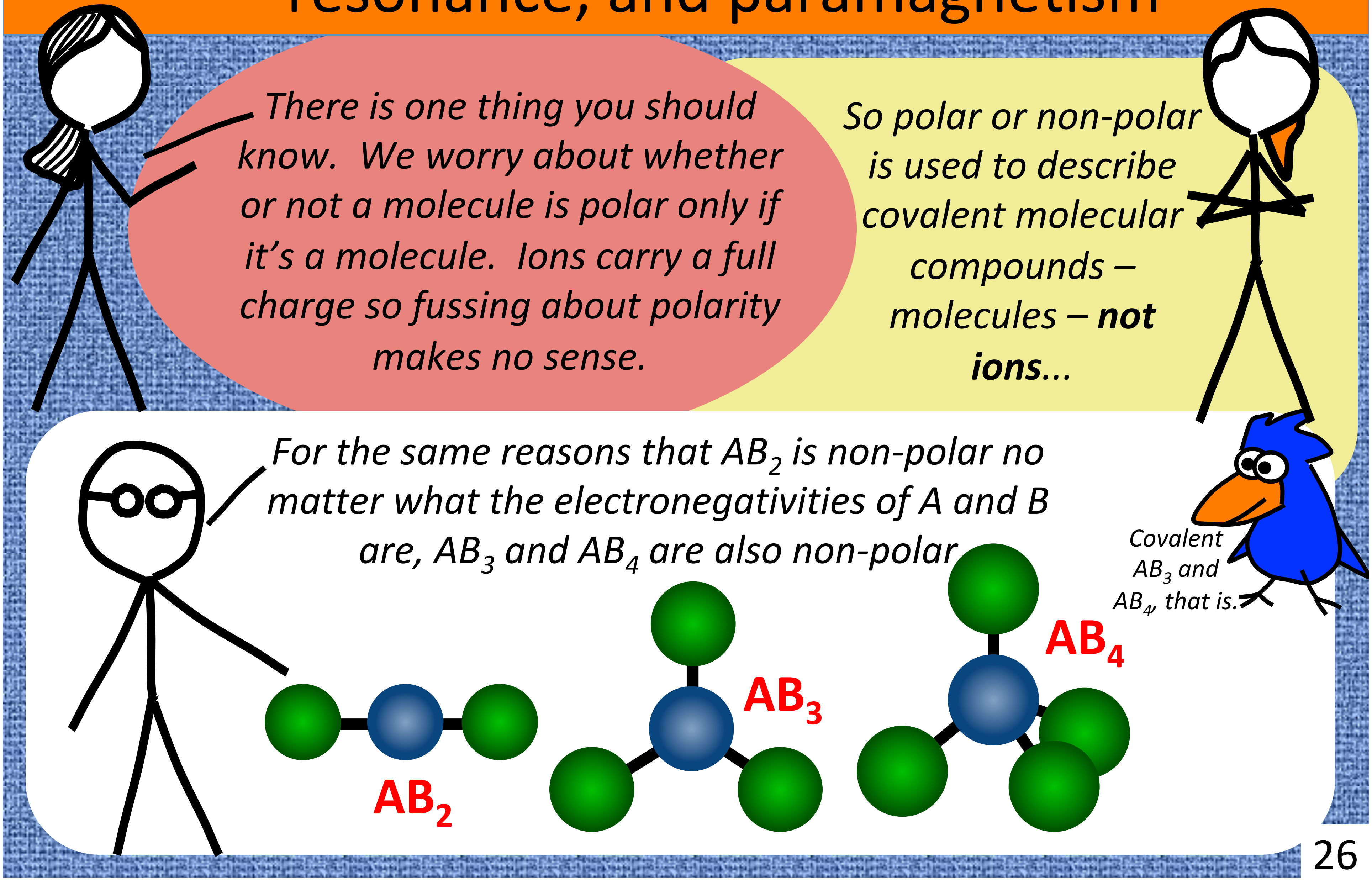
$:C:::O:$

ABE *ABE*

3. Molecular polarity, hybridization, resonance, and paramagnetism

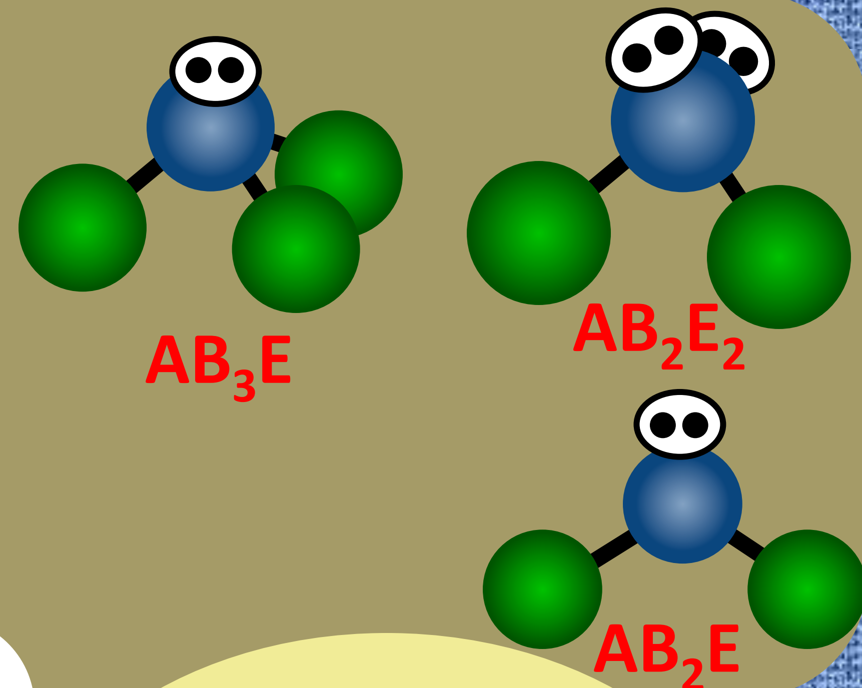


3. Molecular polarity, hybridization, resonance, and paramagnetism

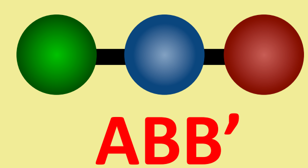


3. Molecular polarity, hybridization, resonance, and paramagnetism

The other three ABE formulas have at least one E group and are polar because the E groups can't offset the polar bonds between A and B.

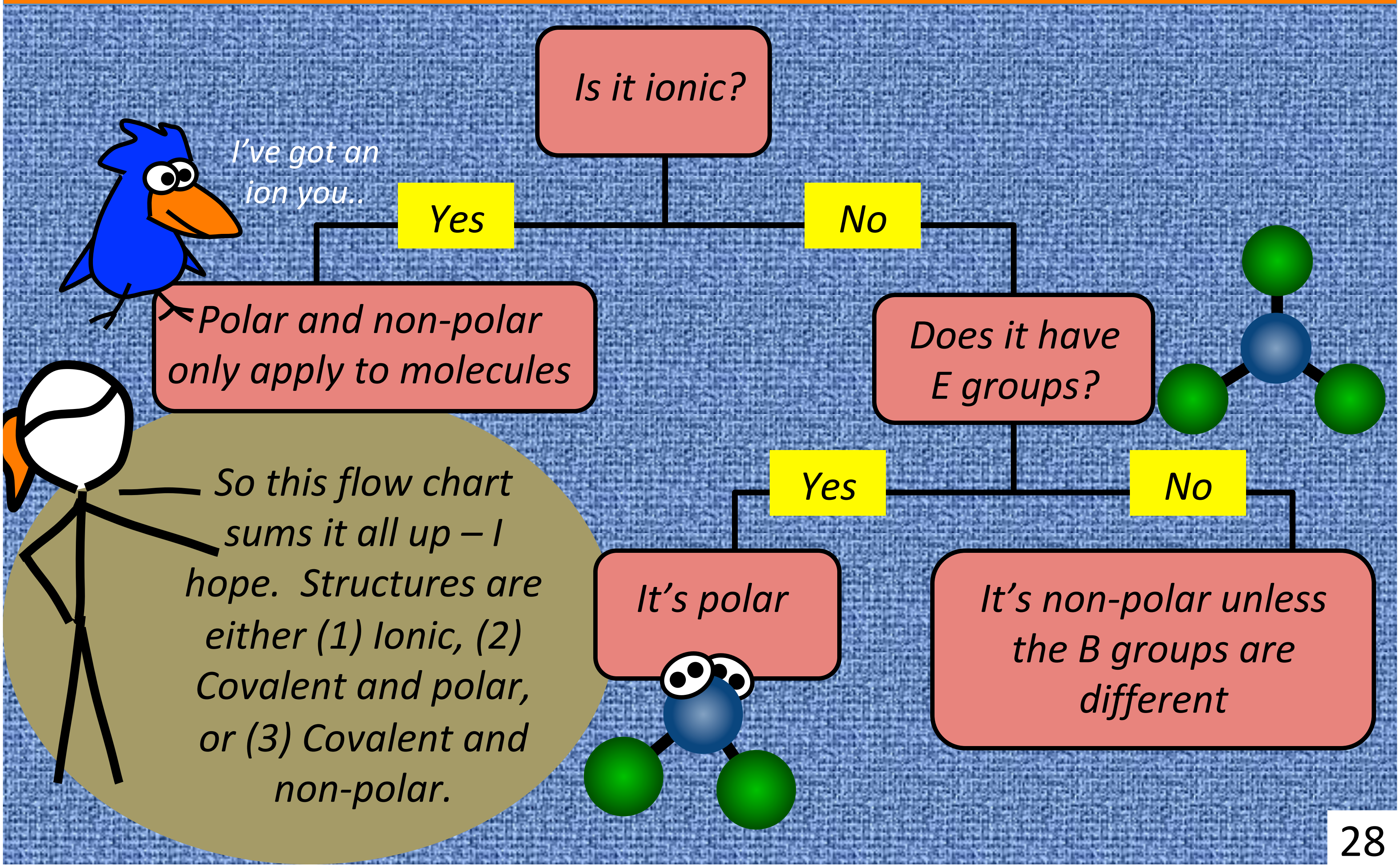


Anything with just two atoms is polar if the atoms are different, for example, CO is polar. Two atom molecules are non-polar if the atoms are the same, for example, O_2.



If B and B' have different electronegativities, this guy is technically polar even without E groups on the central atom

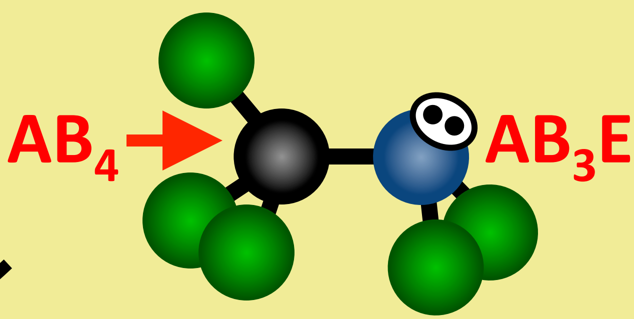
3. Molecular polarity, hybridization, resonance, and paramagnetism



3. Molecular polarity, hybridization, resonance, and paramagnetism

Ok, so far? I'm going to bend your brain just a bit more now… Ready?

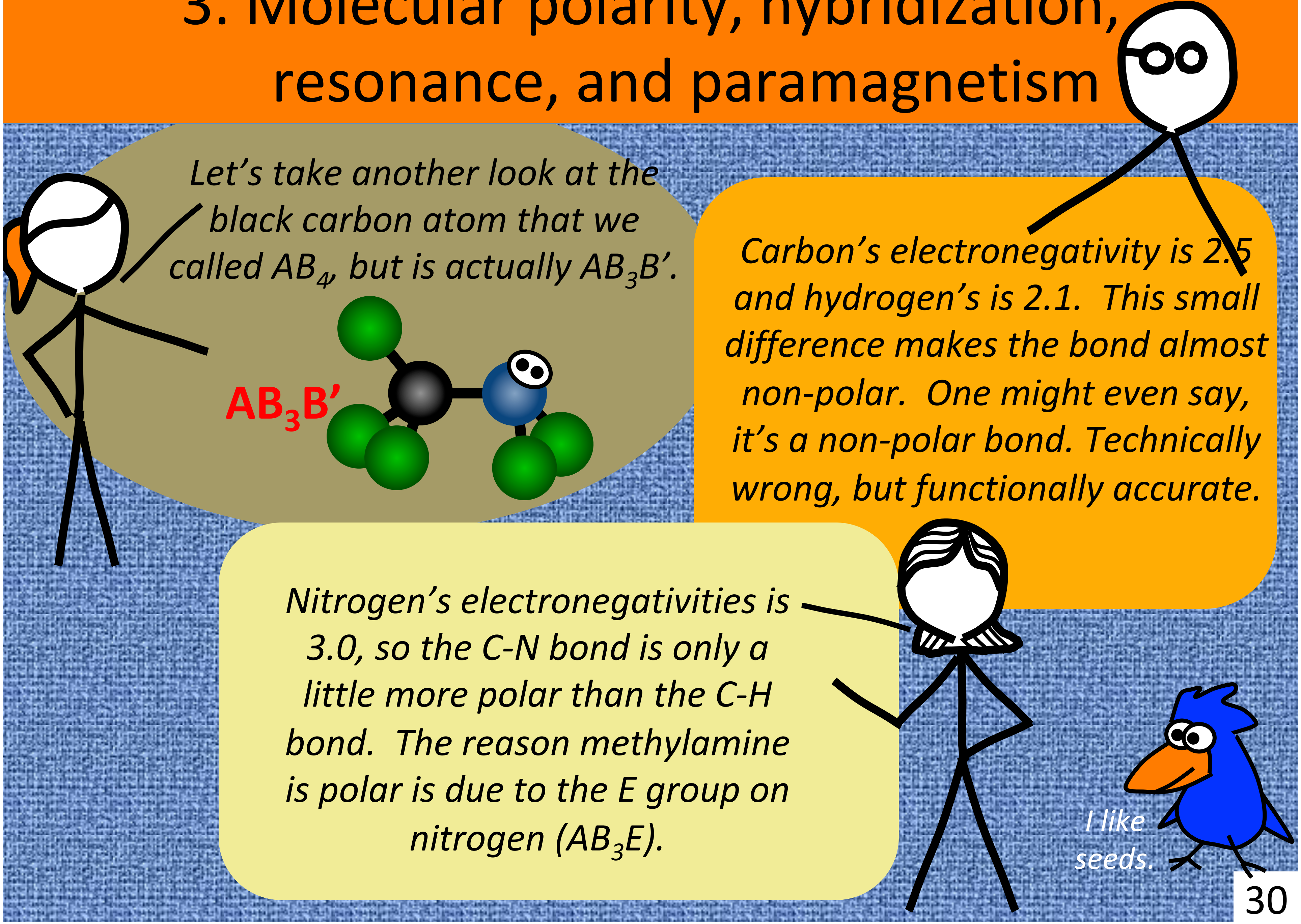
Some molecules have two or more "central atoms." Happens all the time. A simple example is methylamine shown below. It features a carbon atom in black bonded to a nitrogen atom in blue. Green atoms are hydrogen.



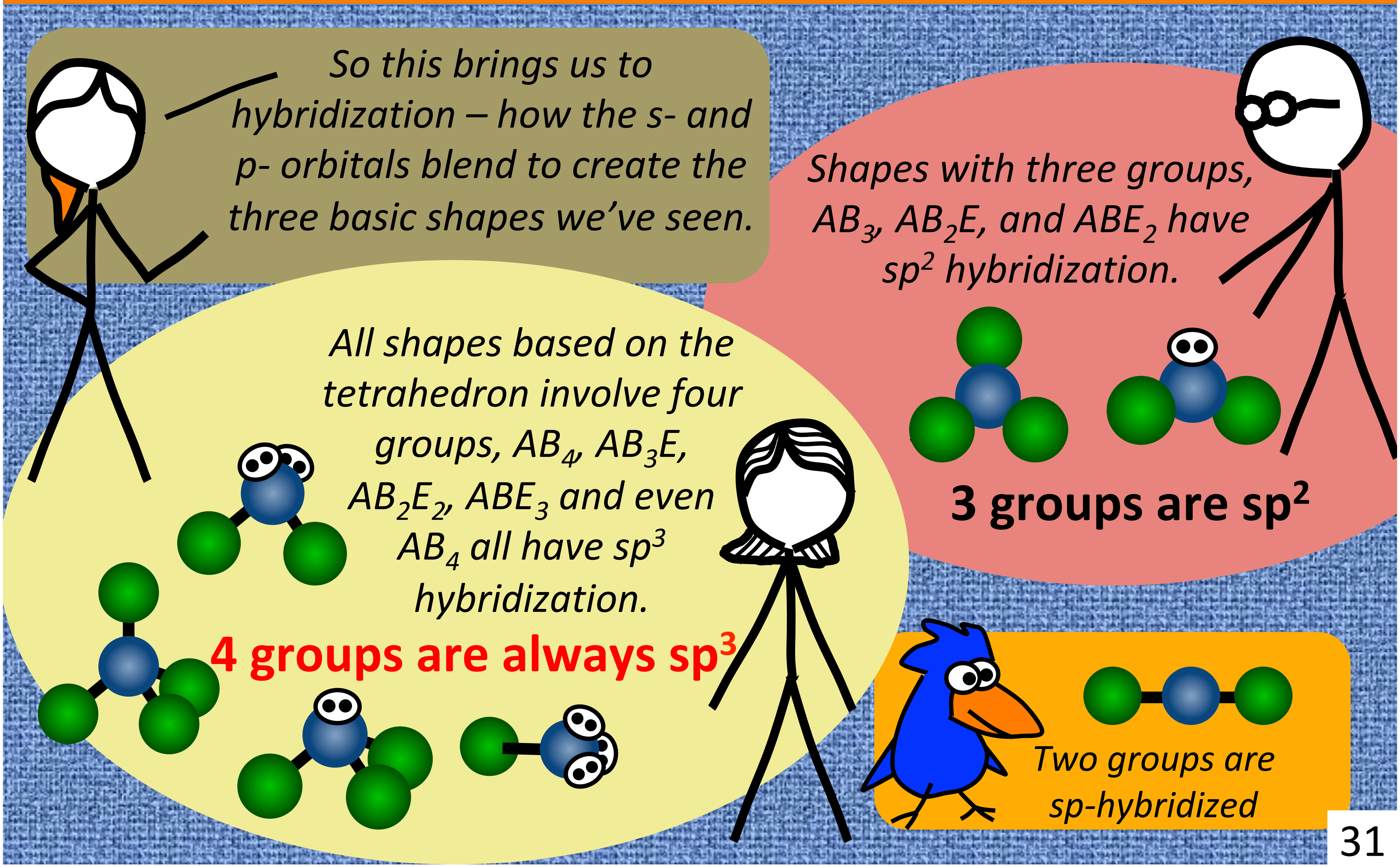
So the carbon atom has no E group, so is essentially non-polar, even though it's technically AB_3B'.

BUT, the nitrogen atom has an E group, making that part of the molecule polar!

3. Molecular polarity, hybridization, resonance, and paramagnetism



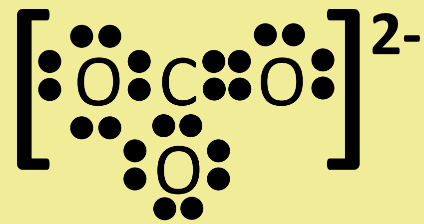
3. Molecular polarity, hybridization, resonance, and paramagnetism



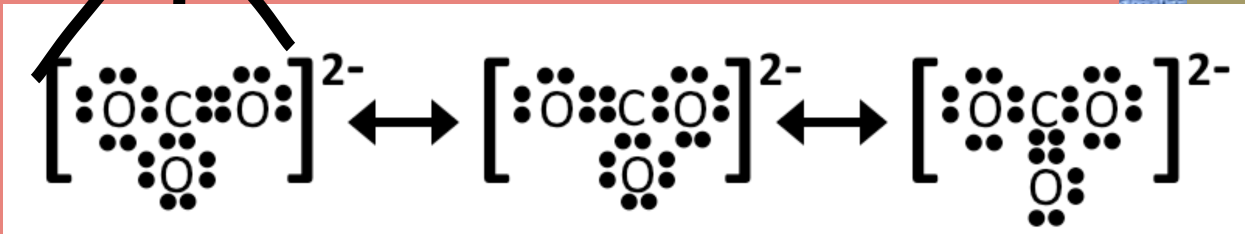
3. Molecular polarity, hybridization, resonance, and paramagnetism

Resonance takes on a variety of forms, but in Gen Chem it is introduced with bonding to oxygen..

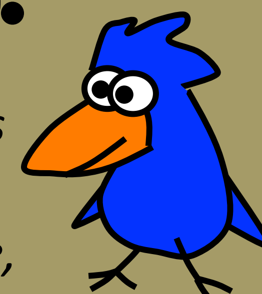
We saw how some molecules made single and double bonds to oxygen – molecules and ions that have both types of bonding to oxygen, have resonance.



Resonance means we need two or more sketches to show how the double bond is shared within the molecule or ion.



Carbonate has resonance. Carbon dioxide, not so much.



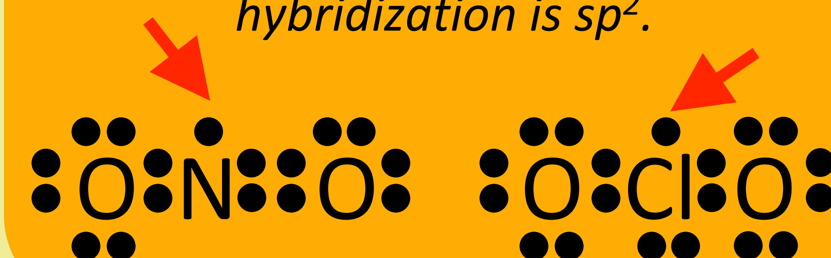
3. Molecular polarity, hybridization, resonance, and paramagnetism

So that brings up paramagnetism. ***Paramagnetism*** *is a term to describe molecules or ions with one or more* ***unpaired*** *electrons*

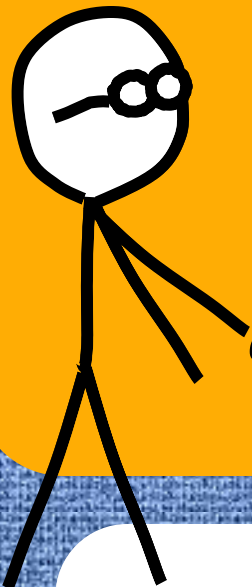
These are weirdoes. All the examples so far have been of molecules with octets with all electrons in pairs, either B or E groups. When every electron is paired, the molecule is called ***diamagnetic****.*

Even though they are few in number, paramagnetic structures are important. Here are two examples. The red arrow points to the unpaired electron.

The molecule NO_2 has one unpaired electron – it still takes up space and so the molecule is AB_2E, so hybridization is sp^2.

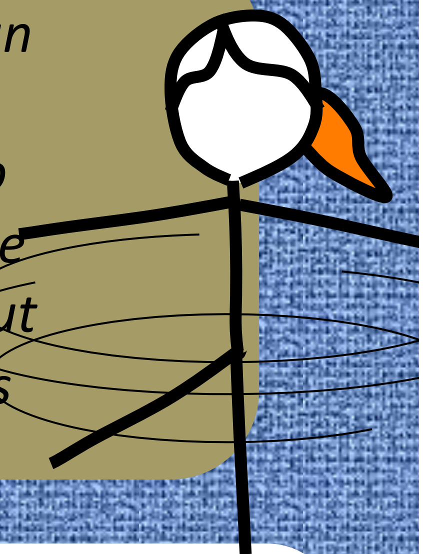


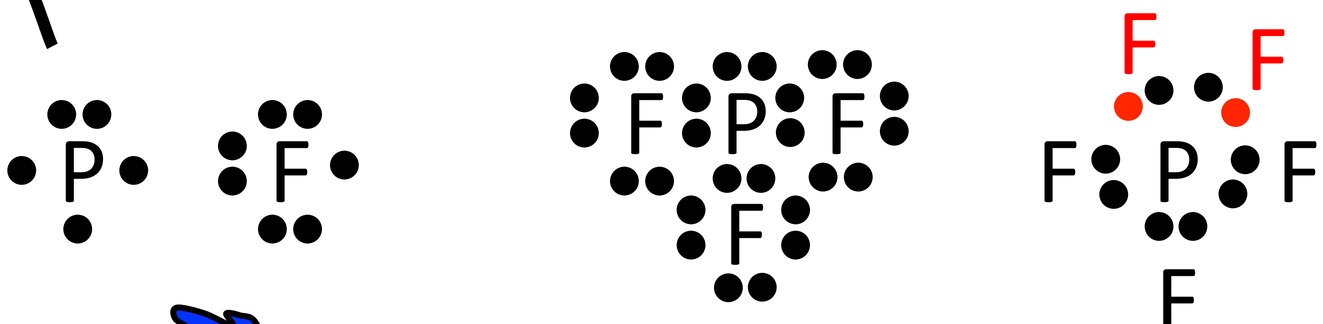
4. Expanded octets



A few compounds and ions have more than 8 electrons around the central atom. This almost always involves fluorine as B groups.

An octet molecule with an E group on the central atom can "expand" into two B groups. That is the easiest way to think about it. One E group becomes two B groups.

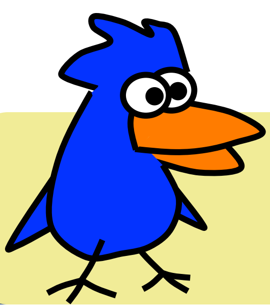




PF_3 is AB_3E

PF_5 is AB_5

E group electrons on F omitted for clarity.

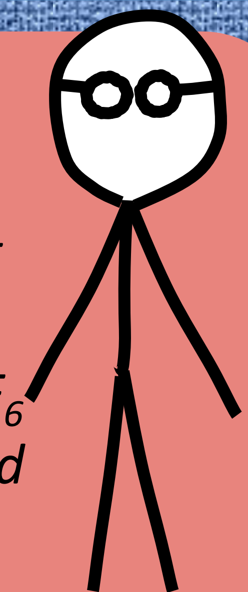


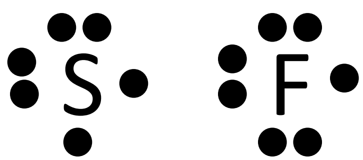
This never ever never happens to second row elements (B, C, N, O, F, and Ne). Never. Ever. And really only happens when the B groups are fluorine.

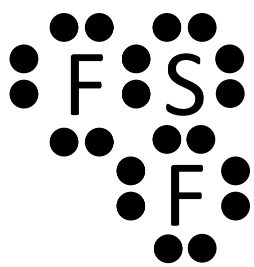
4. Expanded octets

Sulfur difluoride is an octet molecule. It can add another pair of fluorine atoms by expanding an E group (E → 2B).

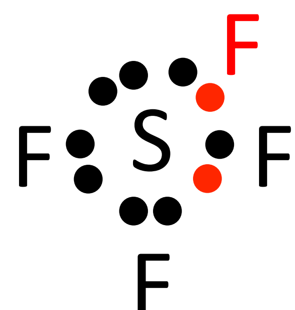
The sulfur atom has "expanded" to 10 electrons between B and E groups. It can do it again because it still has another E group. SF_6 is an important molecule and is AB_6.





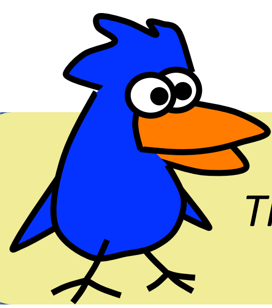


SF_2 is AB_2E_2



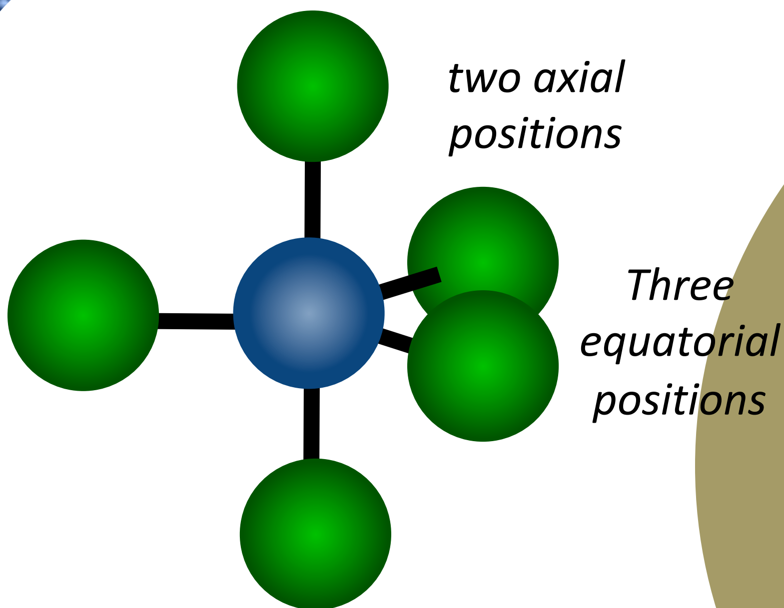
SF_4 is AB_4E

E group electrons on F omitted for clarity.



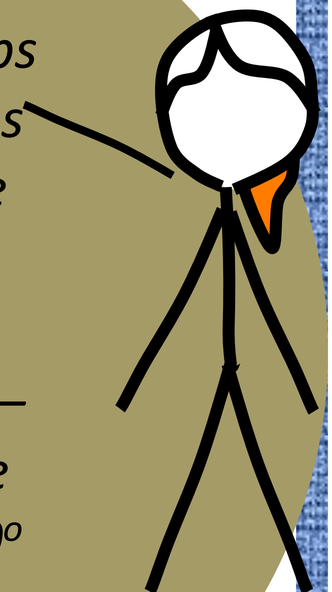
We still use the same three steps to make an octet molecule. Then in a 4th step we expand the octet with E → 2B. Sometimes we can do this twice if there are two E groups.

4. Expanded octets



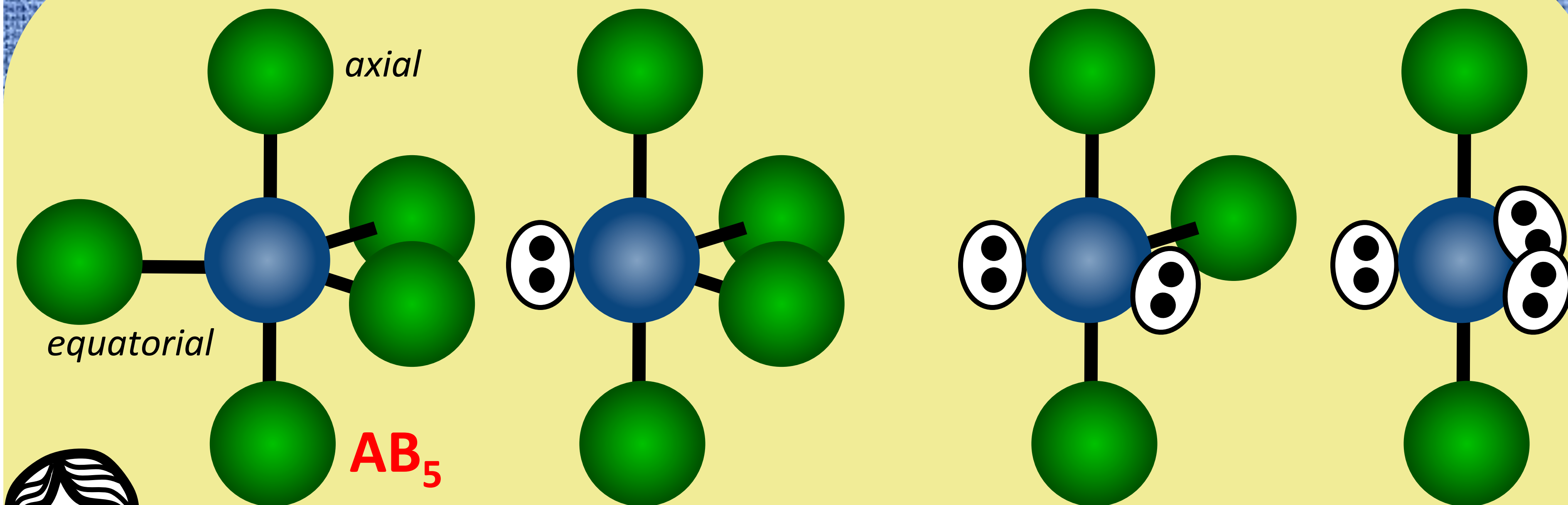
AB_5
trigonal bipyramid

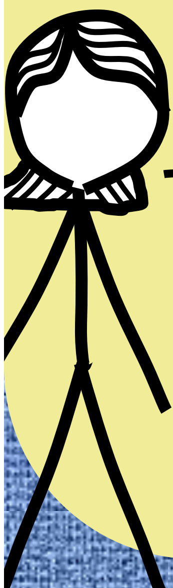
About things with five groups – the trigonal bipyramid has two axial groups and three equatorial groups. The equatorial groups are the same as the trigonal plane – 120^o. The equatorial plane and the axial groups are 90^o apart. Covalent molecules that are AB_5 such as PF_5 are non-polar.



We can't sketch a 5-member geometry in which all five things are the same.

4. Expanded octets





The trigonal bipyramid is AB_5 and is non-polar. The other 5 group possibilities are summarized here.

AB_4E
see-saw
polar

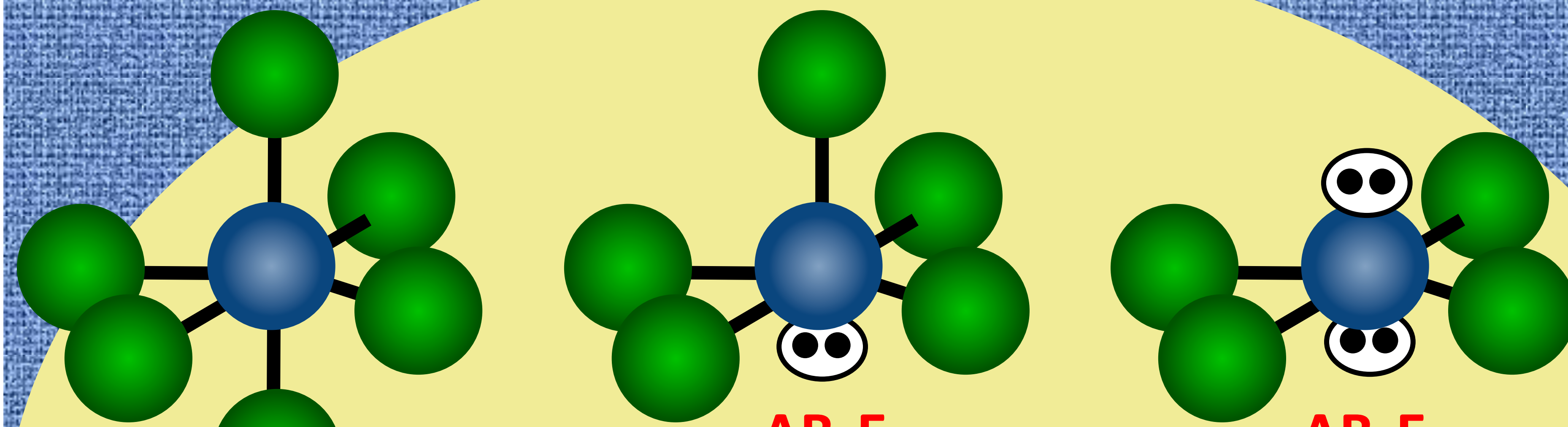
AB_3E_2
T-shaped
polar

AB_2E_3
linear
non-polar

Alert!

Even though AB_2E_3 has E groups, it is non-polar. Gotta love geometry!

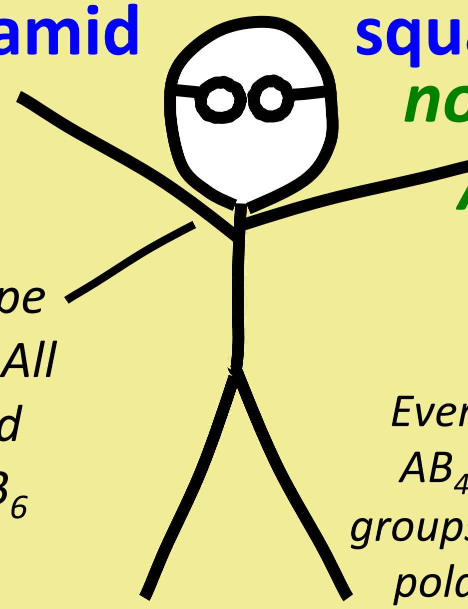
4. Expanded octets



AB_6
octahedral
non-polar

AB_5E
square pyramid
polar

AB_4E_2
square plane
non-polar
Alert!

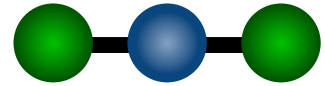


Six groups take the shape of the octahedron, AB_6. All the angles are 90° (and 180°). All molecular AB_6 are non-polar.

Even though AB_4E_2 has E groups, it is non-polar. Why?

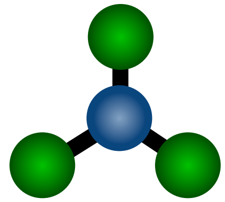
5. Summary

2 Groups = sp (180°)

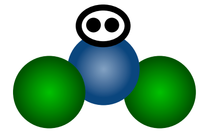


AB_2 linear, non-polar

3 Groups = sp^2 (120°)



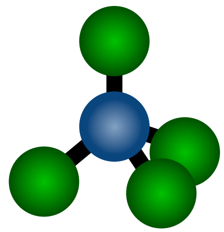
AB_3 trigonal plane, non-polar



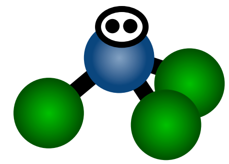
AB_2E bent, polar

Polar and non-polar refer to covalent molecules with identical B groups. Ionic structures are… ionic.

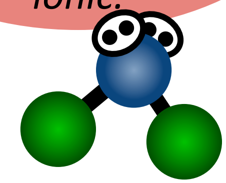
4 Groups = sp^3 (109°)



AB_4 tetrahedral, non-polar

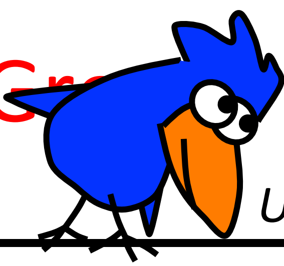


AB_3E trig pyramid, polar

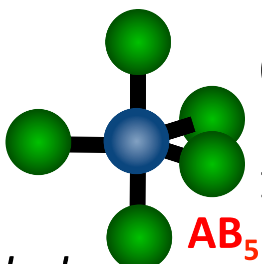


AB_2E_2 bent, polar

5 Gr

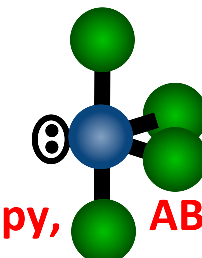


Uh-huh.



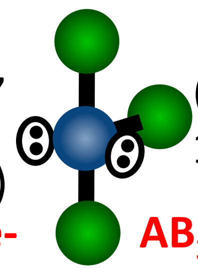
(90°, 120°, 180°)

AB_5 trig bipy, non-polar



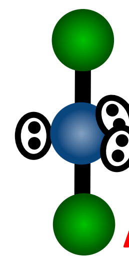
(90°, 120°, 180°)

AB_4E see-saw, polar



(90°, 180°)

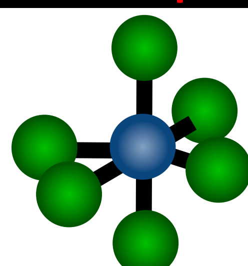
AB_3E_2 T-shaped, polar



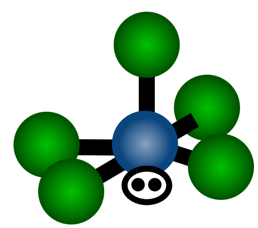
(180°)

AB_2E_3 linear, non-polar

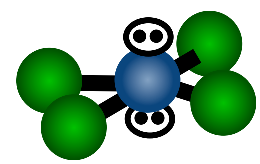
6 Groups (90° and 180°)



AB_6 octahedral, non-polar



AB_5E sq pyramid, polar



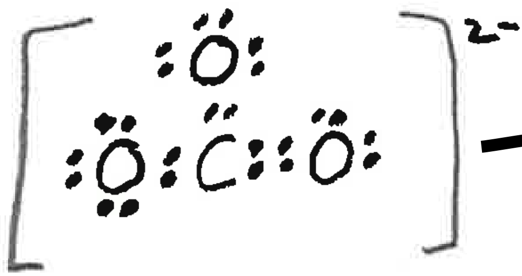
AB_4E_2 sq plane, non-polar

5. What we do today

From the Lewis dot structure, we get the ABE formula and the ABE formula gives us shape, angles and hybridization.

1. Compound/Ion: CO_3^{-2}

(1.0 pt) Correct Lewis structure (no partial credit):



(0.5 pts) ABE formula: AB_3

(0.5 pts) Shape name: trigonal plane

(0.3 pts) Angles: ☐ 90° ☐ 109° ■ 120

(0.3 pts) Hybridization: ☐ sp ■ sp^2

(0.2 pts) Best: ■ Ionic ☐ Polar CM ☐

(0.1 pts) Resonance? ■ Yes ☐ No

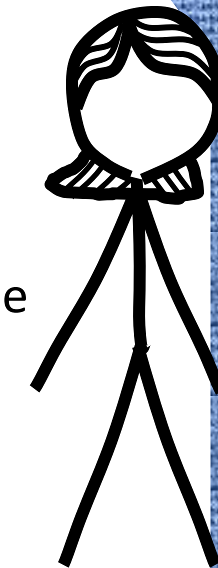
(0.1 pts) Paramagnetic? ☐ Yes ■ No

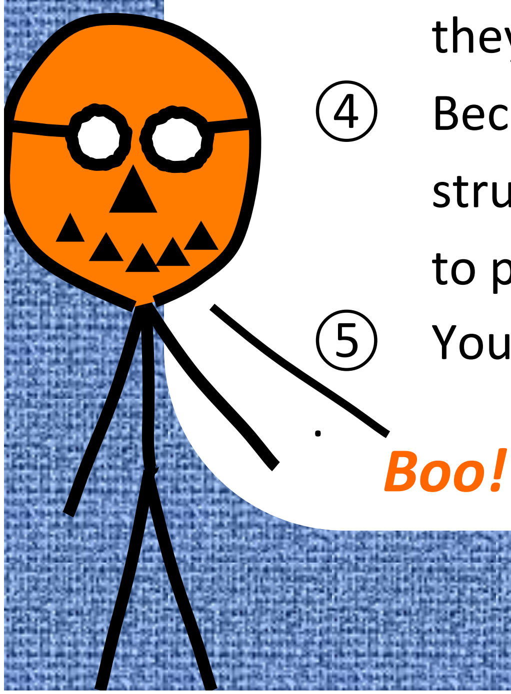
We'll each be doing 16 structures today such as the carbonate ion. Start with a carefully drawn Lewis structure. Follow the three step approach presented in Slides 8 - 15.

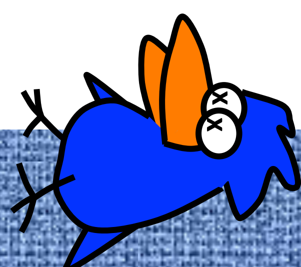
Remember polar and non-polar refer to covalent molecules only. Ionic structures are… ionic. So we would check ***Ionic*** *for CO_3^{2-} even though it is AB_3. This BEST describes how it behaves in solid and solution.*

5. What we do today

1. Safety rules for today: No running with scissors.
2. This is not a normal lab with a lab report. There is no need to write stuff in your lab notebook.
3. Build models of the basic molecular shapes, AB_2, AB_3, AB_4, AB_5, and AB_6. The subsets such as AB_3E can be made from AB_4 – by removing one B group. In the models, we don't't' represent the E groups but we can "see" where they are by the shape they help create.
4. Become competent correctly drawing Lewis dot structures and turning them into ABE formulas in order to predict shape.
5. You will turn in your worksheet before you leave today.







Stick people inspired by xkcd cartoons by Randall Munroe (www.xkcd.com)

Chem Lab with the Stick People and Bird *was created and produced by Dr. Bruce Mattson, Creighton Chemistry. Enjoy it and share it if you wish.*