CHEM 115
Lewis Structures Model
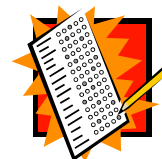
Lecture 22
Prof. Sevian

Please see "Important Announcements" slide inside for more details on the following:

Exam 3 is postponed to May 6 in order to give you the opportunity to use the post-test during lab the week of April 28 as a practice for Exam 3 as well as the final exam.

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Important announcements

Exam 3 is postponed to Tuesday May 6 because…

Test at the beginning of Lab 10 next week (week of April 28)

- Your TA's will bring you to a classroom (it is W-2-198 in case you're late)
- Students who are not enrolled in lab should go to the first hour of one of the lab sections next week (Mon 12:30, Tues 9AM or Weds 12:30) – if that is not possible, then please email me (hannah.sevian@umb.edu) to set up a time next week to take the test
- This is a post-test. It is matched to the pre-test you took at the beginning of the semester.
- Value of the test for you:
  - Offers practice with ACS multiple choice. You will receive the tests back on Thursday May 1 and I will post answers. Studying how you did on it can help you prepare for Exam 3 and the ACS final exam.
  - I will analyze your post-test scores and will give each student a personalized "academic prescription" for the types of problems you most need to study for the final exam. I will give this to you on the last day of class (May 13).
  - Everyone who takes the test will receive 10 points (attendance).
  - I will also compute the pretest-to-posttest change for each person and will give everyone between 1 and 5 extra credit points based on individual potential improvement. Thus, it is to your advantage to try to do well on the posttest.

Agenda

- Find your groups
- Turn in Group Problem #7 by 2:40
- Go over group problem in class
- Power of the Lewis structure model for predicting
  - Bonding arrangements in molecular compounds
  - Bond length and bond strength
    - Single, double, triple
    - Fractional with resonance structures
  - Stability of a structure using formal charges as a guide

- Final Exam has been scheduled for:
  Wednesday, May 21
  8:00-11:00AM
  Snowden Auditorium (W-1-88)
  Please let me know by Friday, April 25, if you have any conflicts with other course's final exams

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Building Lewis Structures

1. Determine central atom (atom with lowest electron affinity because electron density will spread as far as possible, given the opportunity)

2. Count total number of valence electrons in molecule

3. Arrange atoms around central atom

4. Start with single bonds

5. Place remaining valence electrons

6. Move electrons to form octets, making double or triple bonds where necessary

Check: Make sure you have conservation of electrons

Group Problem #7

Draw these Lewis structures:

a) NO_2^+

b) CN^-

c) SCN^-

d) O_3

Then answer the following two questions:

1. Which two of the above structures are isoelectronic?

2. What do you notice that is special about isoelectronic species?

You will need the following definition:
Isoelectronic = same number of (valence) electrons and
same number of atoms to distribute them around

(space for you to take notes on solution to group problem)

Practicing the Steps

Draw the Lewis structure for the nitrate ion (NO_3^-)

1. N is central because it has the least electron affinity
2. Total valence electrons
   - 5 on N
   - 6 on each of three O atoms gives 18 more
   - Ion has -1 charge, meaning one electron is added
   - Total = 5 + 18 + 1 = 24

The rest of the steps:

## Predictions that can come from Lewis structures

- Resonance
- Bond order (useful for comparing strengths of bonds)
- Bond length comparisons (comparing one molecule to another)
- Formal charge (useful for predicting which resonance structures are most stable)

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$$Bond\ order = \frac{\#\ of\ bonds}{\#\ of\ locations}$$

Resonance Structures
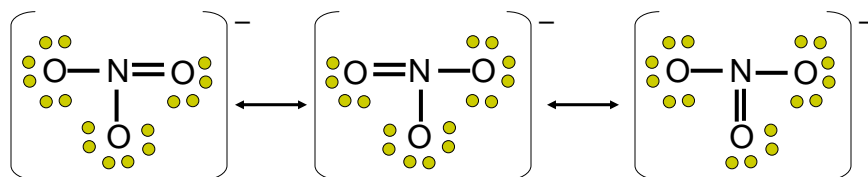
- What do these structures have in common?

- How are they different?

- Which of these is the actual structure of NO_3^-?

Average bond order = 4 bonds split over 3 locations = 4/3
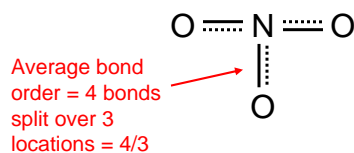
Note: This is not a correct Lewis structure. It is drawn this way _only_ to emphasize the bond order.

Bond Order and Bond Length/Strength

- Bond order
  - Single bond is bond order 1
  - Double bond is bond order 2
  - Triple bond is bond order 3
  - Fractional bond orders occur when there are resonance structures

Average bond order = 4 bonds split over 3 locations = 4/3

- Bond strength
  - The greater the bond order, the stronger the bond (the more energy required to break the bond)
- Bond length
  - The greater the bond order, the shorter the bond length

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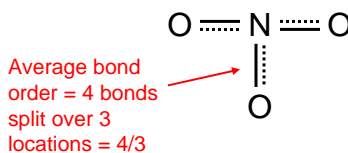
Bond strength

TABLE 8.4   Average Bond Enthalpies (kJ/mol)

Single Bonds

C—H	413	N—H	391	O—H	463	F—F	155
C—C	348	N—N	163	O—O	146		
C—N	293	N—O	201	O—F	190	Cl—F	253
C—O	358	N—F	272	O—Cl	203	Cl—Cl	242
C—F	485	N—Cl	200	O—I	234		
C—Cl	328	N—Br	243			Br—F	237
C—Br	276			S—H	339	Br—Cl	218
C—I	240	H—H	436	S—F	327	Br—Br	193
C—S	259	H—F	567	S—Cl	253		
		H—Cl	431	S—Br	218	I—Cl	208
Si—H	323	H—Br	366	S—S	266	I—Br	175
Si—Si	226	H—I	299			I—I	151
Si—C	301						
Si—O	368						
Si—Cl	464						

Multiple Bonds

C=C	614	N=N	418	O$_2$	495
C≡C	839	N≡N	941		
C=N	615	N=O	607	S=O	523
C≡N	891			S=S	418
C=O	799				
C≡O	1072				

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Bond length

TABLE 8.5   Average Bond Lengths for Some Single, Double, and Triple Bonds

Bond	Bond Length (Å)	Bond	Bond Length (Å)
C—C	1.54	N—N	1.47
C=C	1.34	N=N	1.24
C≡C	1.20	N≡N	1.10
C—N	1.43	N—O	1.36
C=N	1.38	N=O	1.22
C≡N	1.16		
		O—O	1.48
C—O	1.43	O=O	1.21
C=O	1.23		
C≡O	1.13		

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Formal Charges

A comparison between the valence electrons originally contributed by an atom and the electrons that it looks like the atom would have if all bonds were broken and electrons reassigned democratically.

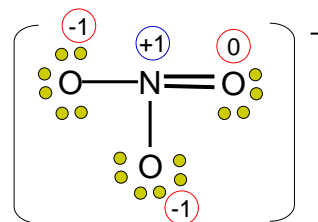The valence electrons that were <u>originally</u> contributed:
- each O had 6
- the N had 5

The formal charges model is used to explain why some resonance structures are more stable than others.

Electrons assigned democratically if bonds hypothetically broken
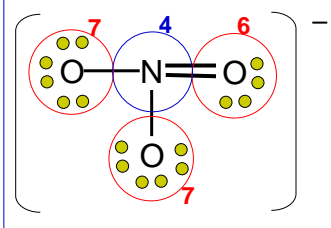
Therefore, the formal charges on each atom are

Notice that the sum of the formal charges must equal the ion charge

Formal Charges and Alternative Structures

- If more than one Lewis structure exists, the most stable structure is the one in which the formal charges make most sense
  - Negative formal charges on atoms with large electron affinity
  - Positive formal charges on atoms with small ionization energies (small electron affinity)
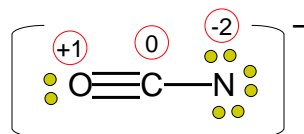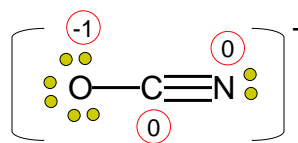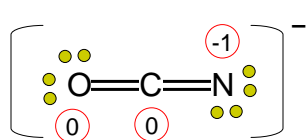
What we have learned today

- Ionic vs. covalent bonding
  - Ionic bond is attraction between + and – ions, held together by Coulomb force of attraction acting across ion separation
  - Molecular bond is valence electrons shared between two atoms and attracted (but not necessarily equally) to both atoms in the bond
- Many aspects of molecular bonding can be modeled by Lewis structures
  - Bond order/strength and length
  - Resonance structures of molecules (or ions) and formal charges on individual atoms in the molecules (or ions)
  - *Bond polarity (not on Exam 3, will be covered on Tuesday)*
  - *Molecular geometry (chapter 9 material, not on Exam 3)*

What is and is not on Exam 3

- Exam 3 covers sections 6.5 through 6.9, and 7.1 through 7.5, and 8.1, 8.2, 8.3, 8.5 and 8.6 in the book. The corresponding homework assignments are 10, 11 and 12. (Homework questions 8.37 and 8.39 from A#12 won't be on Exam 3)
- Section 8.4 will be covered on Tuesday, but it will not be on Exam 3. Sections 8.7 and 8.8 also will not be on Exam 3, but they will be on the final exam.

Where we are going next

- The electronegativity model explains two things:
  - There is a gray area between covalent bonding and ionic bonding: ranging from not polar at all, to so completely polar that the electron transfers completely
  - You can compare the polarities of bonds within molecules, and ultimately you can predict the overall polarity of a molecule (by a vector sum of all the bond polarities in a molecule)

- There are exceptions to the octet rule in Lewis structures
  - Some atoms (notably Be, B and Al) can have less than an octet of electrons and be stable
  - Odd electron molecules are free radicals
  - Atoms that can have more than octet must have *d*-orbitals that can be used to create the beyond-octet options (so the atoms must be at atomic #13 and higher, i.e., having accessible *3d* orbitals and beyond)