

Chemistry 1B Fall 2016

Lectures 10-11-12

Chemistry 1B-AL

Fall 2016

sessions Lectures 10-11-12

1

"Classical" theories of bonding and molecular geometry (ch 13)

- Lewis electron-dot structures
- Bond lengths, energies and ΔH
(back to pp. 615-622, much of this in Chem 1C)
- **Valence State Electron-Pair Repulsion (VSEPR)**
- Polarity of polyatomic molecules (p 600-606)

2

why octets?

filling of ns^2np^6 uses atomic orbitals of similar energy to form covalent bond
(note H requires only 2 electrons)

3

Zumdahl 'steps' (p. 623)

- Sum the valence electrons from all atoms. Do not worry about keeping track of which electrons come from which atoms. It is the *total* number of electrons that is important.
- Use a pair of electrons to form a bond between each pair of bound atoms.
- Arrange the remaining electrons to satisfy the duet rule for hydrogen and the octet rule for the second (and higher) row atoms.

4

how to get octet Lewis structures

Gene's pathetic method:

- use atomic Lewis valence electron diagrams (LVEDs)
- mess around to get octet structures

	1A(1) <i>ns¹</i>	2A(2) <i>ns²</i>	3A(13) <i>ns²np¹</i>	4A(14) <i>ns²np²</i>	5A(15) <i>ns²np³</i>	6A(16) <i>ns²np⁴</i>	7A(17) <i>ns²np⁵</i>	8A(18) <i>ns²np⁶</i>
Period 2	• Li	• Be •	• B •	• C •	• N •	• O •	• F •	• Ne •
Period 3	• Na	• Mg •	• Al •	• Si •	• P •	• S •	• Cl •	• Ar •

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Note from LVEDs (usual bonding configurations to give complete shells)

	1A(1) <i>ns¹</i>	2A(2) <i>ns²</i>	3A(13) <i>ns²np¹</i>	4A(14) <i>ns²np²</i>	5A(15) <i>ns²np³</i>	6A(16) <i>ns²np⁴</i>	7A(17) <i>ns²np⁵</i>	8A(18) <i>ns²np⁶</i>
Period 2	• Li	• Be •	• B •	• C •	• N •	• O •	• F •	• Ne •
Period 3	• Na	• Mg •	• Al •	• Si •	• P •	• S •	• Cl •	• Ar •

- H atom shares 1 pair of e's (peripheral or 'terminal' atom)
- C atom shares 4 pairs of e's
- N atom shares 3 pairs of e's and has 1 non-bonding pair of e's
- O atom shares 2 pairs of e's and has 2 non-bonding pairs of e's
sometimes O-sharing 1 pair of e's and 3 non-bonding pairs
- F atom shares 1 pair of e's and has 3 non-bonding pairs of e's (peripheral or 'terminal' atom)
- similar for period 3 atoms

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examples for molecules with single bonds

- Example 13.6e (p. 625) CF_4
- NH_2^-
- CH_3OH
- $\text{C}_2\text{H}_6\text{O}$ (structural isomers)
 $(\text{CH}_3\text{OCH}_3)$
 $(\text{CH}_3\text{CH}_2\text{OH})$

7

Multiple bonds

Multiple bonds

If, after step sharing single pairs of electrons a central atom still does not have an octet, make a multiple bond by changing a lone pair from one of the surrounding atoms into a bonding pair to the central atom.

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examples

- C_2H_4
- C_2H_2
- COF_2

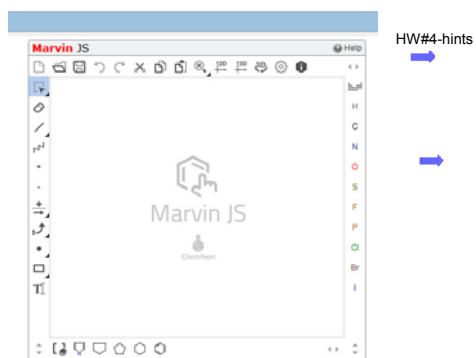
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MASTERING LEWIS STRUCTURES = PRACTICE PRACTICE PRACTICE



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WebAssign and Marvin JS (HW4 #35)



11

Resonance Structures and Formal Charge

(pp 626-627, 631-634)

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covered worksheet VI 1.1-1.5

Learning Objectives and Worksheet VI
Chemistry 1B, Fall 2016

Learning Objectives (LOs) for Molecular Structure and Geometry (part I)

LO 1: Lewis Structures (LO 1.1-1.5)

1. Lewis molecular structure

a. Draw Lewis structures for molecules and ions.

b. Determine the number of valence electrons in a molecule or ion.

c. Determine the number of valence electrons in a molecule or ion.

d. Determine the number of valence electrons in a molecule or ion.

e. Determine the number of valence electrons in a molecule or ion.

f. Determine the number of valence electrons in a molecule or ion.

g. Determine the number of valence electrons in a molecule or ion.

h. Determine the number of valence electrons in a molecule or ion.

i. Determine the number of valence electrons in a molecule or ion.

j. Determine the number of valence electrons in a molecule or ion.

k. Determine the number of valence electrons in a molecule or ion.

l. Determine the number of valence electrons in a molecule or ion.

m. Determine the number of valence electrons in a molecule or ion.

n. Determine the number of valence electrons in a molecule or ion.

o. Determine the number of valence electrons in a molecule or ion.

p. Determine the number of valence electrons in a molecule or ion.

q. Determine the number of valence electrons in a molecule or ion.

r. Determine the number of valence electrons in a molecule or ion.

s. Determine the number of valence electrons in a molecule or ion.

t. Determine the number of valence electrons in a molecule or ion.

u. Determine the number of valence electrons in a molecule or ion.

v. Determine the number of valence electrons in a molecule or ion.

w. Determine the number of valence electrons in a molecule or ion.

x. Determine the number of valence electrons in a molecule or ion.

y. Determine the number of valence electrons in a molecule or ion.

z. Determine the number of valence electrons in a molecule or ion.

AA. Determine the number of valence electrons in a molecule or ion.

AB. Determine the number of valence electrons in a molecule or ion.

AC. Determine the number of valence electrons in a molecule or ion.

AD. Determine the number of valence electrons in a molecule or ion.

AE. Determine the number of valence electrons in a molecule or ion.

AF. Determine the number of valence electrons in a molecule or ion.

AG. Determine the number of valence electrons in a molecule or ion.

AH. Determine the number of valence electrons in a molecule or ion.

AI. Determine the number of valence electrons in a molecule or ion.

AJ. Determine the number of valence electrons in a molecule or ion.

AK. Determine the number of valence electrons in a molecule or ion.

AL. Determine the number of valence electrons in a molecule or ion.

AM. Determine the number of valence electrons in a molecule or ion.

AN. Determine the number of valence electrons in a molecule or ion.

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AW. Determine the number of valence electrons in a molecule or ion.

AX. Determine the number of valence electrons in a molecule or ion.

AY. Determine the number of valence electrons in a molecule or ion.

AZ. Determine the number of valence electrons in a molecule or ion.

BA. Determine the number of valence electrons in a molecule or ion.

BB. Determine the number of valence electrons in a molecule or ion.

BC. Determine the number of valence electrons in a molecule or ion.

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BE. Determine the number of valence electrons in a molecule or ion.

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BG. Determine the number of valence electrons in a molecule or ion.

BH. Determine the number of valence electrons in a molecule or ion.

BI. Determine the number of valence electrons in a molecule or ion.

BJ. Determine the number of valence electrons in a molecule or ion.

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BL. Determine the number of valence electrons in a molecule or ion.

BM. Determine the number of valence electrons in a molecule or ion.

BN. Determine the number of valence electrons in a molecule or ion.

BO. Determine the number of valence electrons in a molecule or ion.

BP. Determine the number of valence electrons in a molecule or ion.

BQ. Determine the number of valence electrons in a molecule or ion.

BR. Determine the number of valence electrons in a molecule or ion.

BS. Determine the number of valence electrons in a molecule or ion.

BT. Determine the number of valence electrons in a molecule or ion.

BU. Determine the number of valence electrons in a molecule or ion.

BV. Determine the number of valence electrons in a molecule or ion.

BW. Determine the number of valence electrons in a molecule or ion.

BX. Determine the number of valence electrons in a molecule or ion.

BY. Determine the number of valence electrons in a molecule or ion.

BZ. Determine the number of valence electrons in a molecule or ion.

CA. Determine the number of valence electrons in a molecule or ion.

CB. Determine the number of valence electrons in a molecule or ion.

CC. Determine the number of valence electrons in a molecule or ion.

CD. Determine the number of valence electrons in a molecule or ion.

CE. Determine the number of valence electrons in a molecule or ion.

CF. Determine the number of valence electrons in a molecule or ion.

CG. Determine the number of valence electrons in a molecule or ion.

CH. Determine the number of valence electrons in a molecule or ion.

CI. Determine the number of valence electrons in a molecule or ion.

CJ. Determine the number of valence electrons in a molecule or ion.

CK. Determine the number of valence electrons in a molecule or ion.

CL. Determine the number of valence electrons in a molecule or ion.

CM. Determine the number of valence electrons in a molecule or ion.

CN. Determine the number of valence electrons in a molecule or ion.

CO. Determine the number of valence electrons in a molecule or ion.

CP. Determine the number of valence electrons in a molecule or ion.

CQ. Determine the number of valence electrons in a molecule or ion.

CR. Determine the number of valence electrons in a molecule or ion.

CS. Determine the number of valence electrons in a molecule or ion.

CT. Determine the number of valence electrons in a molecule or ion.

CU. Determine the number of valence electrons in a molecule or ion.

CV. Determine the number of valence electrons in a molecule or ion.

CU. Determine the number of valence electrons in a molecule or ion.

CV. Determine the number of valence electrons in a molecule or ion.

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MASTERING LEWIS STRUCTURES = PRACTICE PRACTICE PRACTICE

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this video (clickers Q's next class) cover: **worksheet VI II.1-2** and

RESONANCE STRUCTURES

1. Resonance structures

a. All resonance structures of a molecule have identical stoichiometric formulae; all isomeric structures of a molecule have identical stoichiometric formulae. What is the distinction between the meaning of different resonance structures and different isomeric structures?

b. What experimentally measured property would distinguish between C_4H_6 , existing as a mixture of the two structures below and as a resonance hybrid of the structures?

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this video (clickers Q's next class) cover: **and worksheet VI III.1-5**

FORMAL CHARGE

1. Formal charge

a. Formal is concept for assigning net charges to the atoms in a molecule. I first "strip" off the valence electrons leaving positively charged atomic centers and then returns negatively charged valence electrons to the various atoms.

b. For the following atoms what would be their 'starting' positive charge contribution to the formal charge on the atom:

i. B = \dots

ii. N = \dots

iii. P = \dots

iv. O = \dots

v. Br = \dots

2. The negative charges 'valence' electrons are then distributed among the atoms with the following conventions:

3. A non-bonding pair of electrons is assigned to \dots making a contribution of \dots to that atom's formal charge.

4. For each pair of electrons by two atoms, the assignment is \dots making a contribution of \dots to each atoms formal charge.

5. The sum of formal charges must \dots to the \dots on the molecule or molecular ion.

6. We saw that when a molecule has two "equivalent" octet structures, the resulting resonance hybrid is an average structure with equal contributions from the two Lewis structures. More generally, if there are several, but non-equivalent, octet structures that can be drawn for a given molecule, the resulting hybrid will be a weighted average of the possible octet structures. What three factors will determine the best Lewis structures, i.e. the Lewis structures that will dominate (contribute most strongly) to the weighted average hybrid?

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the structure of ozone O_3 but first: the good and the bad

GOOD OZONE
Stratosphere
absorbs sun's harmful ultra-violet radiation

BAD OZONE
Troposphere
produced by photochemical smog; oxidizes materials like lungs and tires

Ozone in the stratosphere protects Earth but in the troposphere, it is harmful.

UCAR©2003

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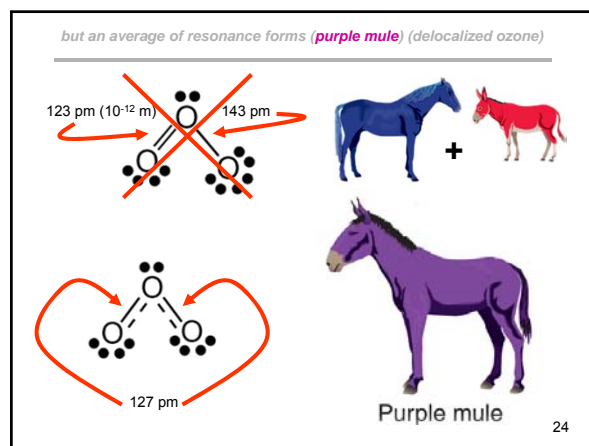
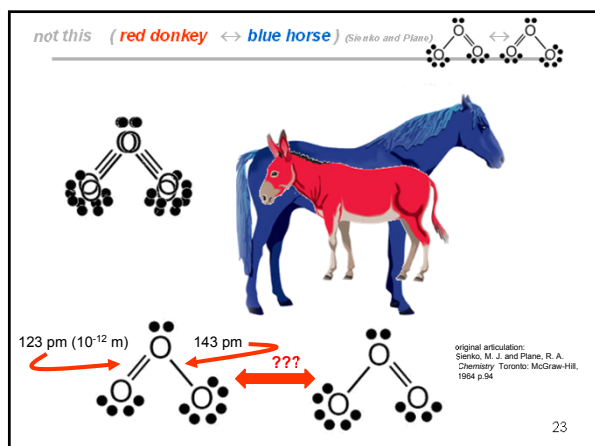
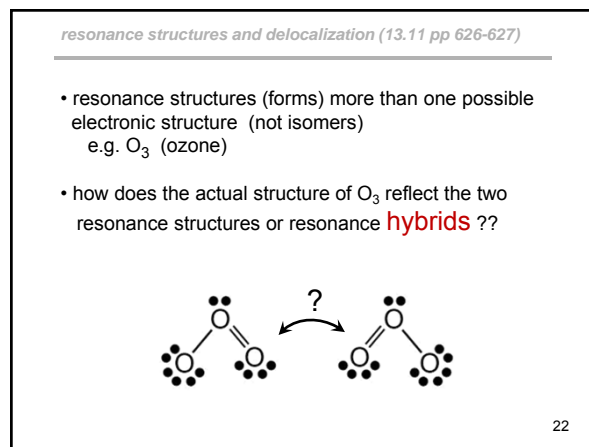
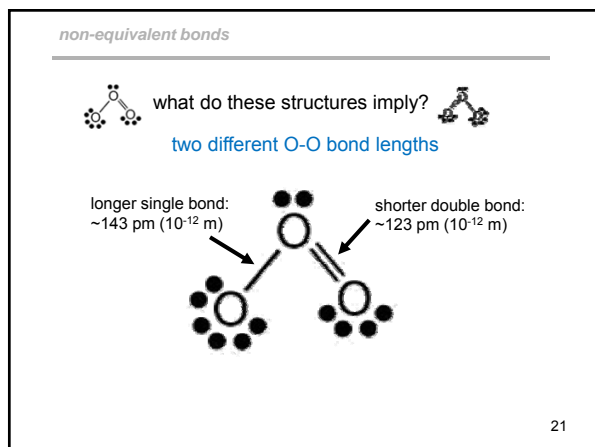
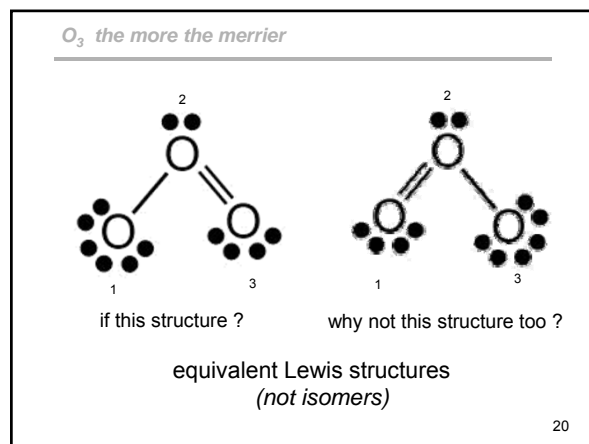
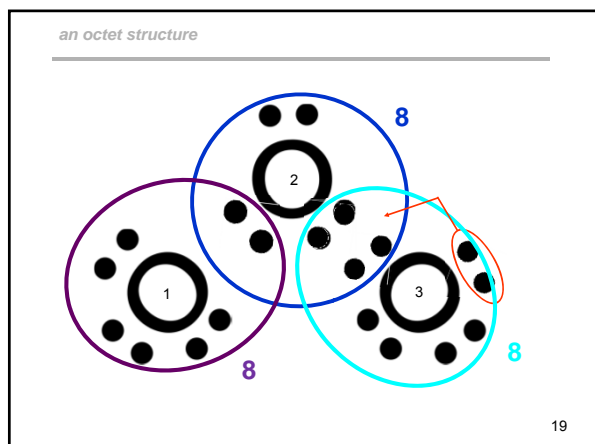
ozone (octet structure)

triangular ??, however, not the most 'stable' structure of O_3 more later

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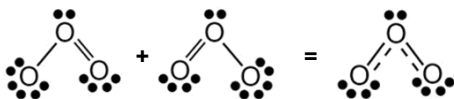


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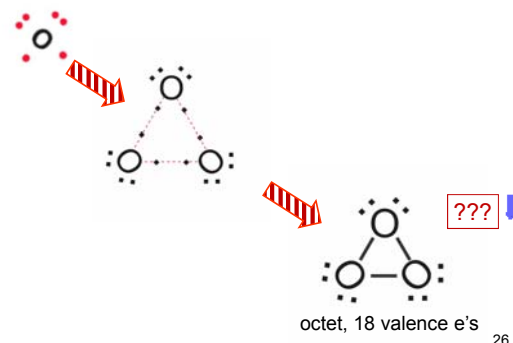
resonance structures and delocalization (13.11 pp 626-627)

- resonance structures (forms) are more than one possible electronic structure (not isomers)
e.g. O_3 (ozone)
- actual structure is average (hybrid) of possible resonance structures



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(now is later !!) O_3 ring structure



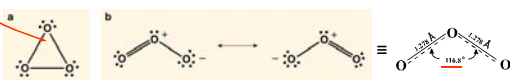
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triangular cyclic O_3

The Story of O
Roald Hoffmann

So now we have oxygen chemistry in the atmosphere, in the cell, in a decontamination process. But have we exhausted all of oxygen's secrets?
<http://www.americanscientist.org/issues/pub/the-story-of-o3> This Article from Issue January-February 2004

60° bond angles are "strained" (unstable);
[discuss later in term (quantum mechanics)]



Indeed, the best calculations today confirm the metastability of this ring. Cyclic ozone lies about **130 kilojoules per mole above normal O_3** but has a barrier of no less than 95 kilojoules per mole preventing conversion to the open form.

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examples of resonance structures

- $[CO_3]^{2-}$ →
- C_6H_6 (in class)

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formal charge on an atom in a molecule:

Formal charge is a way of associating electrons in a molecule with the various atoms thus allowing one to calculate the (approximate) net charge on the atom.

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formal charge on an atom in a molecule:

Conceptual steps:

- remove each atom's valence electrons leaving a residual positive 'core' charge on the atom;
e.g. H^+ , N^{+5} , O^{+6} , etc
- the total negative charge assigned to each atom arises from:
 - electrons in each covalent bond are divided equally between the atoms forming the bond
 - electrons in non-bonding pairs are assigned to the atom on which they reside
- the sum of formal charges must equal the total charge on the atom or ion

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formal charge

formal charge = $\begin{matrix} \text{positive core charge} \\ + \text{ \# of valence electrons (in neutral atom)} \end{matrix}$

negative charge from electrons assigned to atom $\begin{cases} - \text{ \# of nonbonding electrons} \\ - \frac{1}{2} \text{ \# of bonding electrons} \end{cases}$

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formal charge vs oxidation number (p 633, p 126)

- formal charge = # of valence electrons (in neutral atom)
 - # of nonbonding electrons
 - $\frac{1}{2}$ # of bonding electrons
- oxidation number = valence electrons
 - nonbonding electrons
 - 'assigned' bonding electrons†

Chem 1A nr

† bonding electrons 'assigned' to more electronegative atom in bond

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formal charge and stability of resonance forms

- for non-equivalent resonance forms, the resonance form is preferable (*makes a greater contribution to the average resonance hybrid*) if it has:
 - small formal charges
 - like charges NOT on adjacent atoms
 - negative formal charges reside on more electronegative atoms
- example : phosgene COCl2

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COCl₂ :phosgene

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COCl₂ : non-equivalent resonance forms

octet structures:

I

II

III

Formal Charge:

O = +6 - 6 - $\frac{1}{2}$ (2) = -1	O = +6 - 4 - $\frac{1}{2}$ (4) = 0	O = -1
C = +4 - 0 - $\frac{1}{2}$ (8) = 0	C = +4 - 0 - $\frac{1}{2}$ (8) = 0	C = 0
Cl = +7 - 4 - $\frac{1}{2}$ (4) = +1	Cl = +7 - 6 - $\frac{1}{2}$ (2) = 0	Cl = 0
Cl = +7 - 6 - $\frac{1}{2}$ (2) = 0	Cl = +7 - 6 - $\frac{1}{2}$ (2) = 0	Cl = +1

+1 on Cl unfavorable *+1 on Cl unfavorable*

II structure with greatest contribution
I and III minor contributions

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Zumdahl Table 2.5 and 13.5, Silberberg figure 9.3

TABLE 13.5 Common Ions with Noble Gas Electron Configurations in Ionic Compounds

Group 1A	Group 2A	Group 3A	Group 6A	Group 7A	Electron Configuration
H ⁺ , Li ⁺	Ba ²⁺		O ²⁻	F ⁻	[He]
Na ⁺	Mg ²⁺	Al ³⁺	S ²⁻	Cl ⁻	[Ar]
K ⁺	Ca ²⁺		Se ²⁻	Br ⁻	[Kr]
Rb ⁺	Sr ²⁺		Te ²⁻	I ⁻	[Xe]
Cs ⁺	Ba ²⁺				

TABLE 2.5 Common Polyatomic Ions

Formula	Name	Charge
NH ₄ ⁺	ammonium	+1
NO ₂ ⁻	nitrite	-1
NO ₃ ⁻	nitrate	-1
SO ₄ ²⁻	sulfate	-2
SO ₃ ²⁻	sulfite	-2
HCO ₃ ⁻	hydrogen carbonate	-1
CO ₃ ²⁻	carbonate	-2
OH ⁻	hydroxide	-1
CN ⁻	cyanide	-1
PO ₄ ³⁻	phosphate	-3
HPO ₄ ²⁻	hydrogen phosphate	-2
H ₂ PO ₄ ⁻	dihydrogen phosphate	-1

KNOW:
 NH₄⁺, NO₃⁻, SO₄²⁻, HSO₄⁻,
 CN⁻, OH⁻, PO₄³⁻, CO₃²⁻,
 HCO₃⁻, C₂H₃O₂⁻, MnO₄⁻

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Marvin JS Resonance Structure (HW#5 37, 44)

Question
RESONANCE STRUCTURE DEMONSTRATION
 (10 submissions)
 Draw Lewis structures for the carbonate anion, [CO₃]²⁻ including resonance forms and formal charges.
 see additional video06a

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Exceptions (13.12 pp 627-636) EXPLAINED BY QUANTUM MECHANICS

- electron deficient atoms: Be, B
 - examples BeH₂ and BF₃
 - quantum mechanics explains
- Free radicals
 - odd number of electrons
 - example CH₃
 - quantum mechanics explains
- 10, 12, 14, 16 electron shells for larger atoms with low-lying d-orbitals
 - structures with 'expanded' shells often have preferable formal charges
 - examples PCl₅, H₂SO₄, [SO₄]²⁻, XeO₄

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HW5 (some of same molecules/ions in each)
 36 **OCTET** (no charges), 39 **OCTET CHARGES**, 40 non-OCTET charges

36. (Zumdahl 13.58 a, c (10 submissions))
 Draw a Lewis structure that obeys the octet rule for each of the following molecules and ions. In each case the first atom listed is the central atom.
 Note that problems 36, 38, and 40 refer to structures for some of the same molecules and ions. Here in HW5 you should just enter the correct structure corresponding to the appropriate number of valence electrons for the molecule or molecular ion, BUT NOT CHARGES ON ATOMS, they come in problem 39!

a. PCl₅

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HW#5 probs 36, 39, 40

Note that problems 36, 38 and 40 refer to structures for some of the same molecules and ions. Here in HW5 you should just enter the correct structure corresponding to the appropriate number of valence electrons for the molecule or molecular ion, BUT NOT CHARGES ON ATOMS, they come in problem 39!

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heads up: very useful handout

CHEMISTRY 1B-AL FALL 2016 HANDOUTS

Course Introduction	Topics Schedule	Homework Assignments	Exams, Objectives, Laboratory & Vespers	Discussion Sections
Course or Materials page	Homework	Topic Based Assignments	HELP resources	no comments on-line Q & A

go to current handouts

HANDOUT	DATE	FORMAT
26 Homework #3	12 Oct	PDF
27 Topic Handouts (9)	17 Oct	PDF(P1) PDF(P2) PDF(P3)
28 Worksheet #5	19 Oct	PDF
29 Homework #4	19 Oct	PDF
30 Topic Handouts (10-12)	19 Oct	PDF(P1) PDF(P2) PDF(P3)
31 Worksheet #6	21 Oct	PDF
32 VSEPR from Dickerson, Gray, Haight	24 Oct	PDF
33 Worksheet #7	26 Oct	PDF
34 Homework #5	26 Oct	PDF
35 Topic Handouts (13-16)	26 Oct	PDF(P1) PDF(P2) PDF(P3)

look at this for VESPER

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back to section 13.8 "bond energies" (616-619)

- the properties (e.g. bond length and bond energy) of localized bonds of a given type are 'somewhat' transferable from molecule to molecule
- one can approximately calculate the relative 'energy' (enthalpy) of a substance by adding the bond energies of its constituent bonds
- since bond energies vary somewhat from compound to compound, we tabulate average bond energies

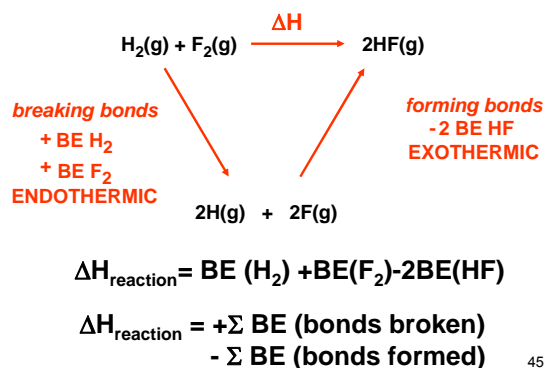
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ARE responsible for: bond lengths and bond energies (qualitative)

- For a given type of covalent bonding (single, double, triple) atomic covalent radius determines bondlength ([figure Silberberg 9.13](#))
- For a given type of atoms the bondlength will be (single) > (double) > (triple) ([Table 13.7](#))
- Bond energies (strengths) will follow the trend (triple) > (double) > (single) ([Table 13.7](#))
- Bond order single b.o.=1, double b.o.=2, triple b.o.=3 (more in chapter 14)

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NOT responsible for: calculating $\Delta H_{\text{REACTION}}$ from bond energies (sec 13.8 \Rightarrow chem 1C)



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TIME TO GET GOING: MIDTERM#2, Nov 9th

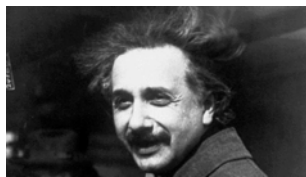


or
else



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Study HINT



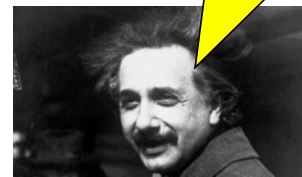
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albert,
tell me,
how is it that you do so
well on your CHEM 1B-02
homework?



Marie Curie

my dear marie,
my secret is that I go to
Ana's sections
and Joselyn's LSS tutorials
and use staff OFFICE HOURS.



Albert Einstein

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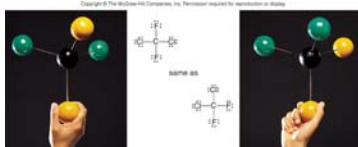
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VSEPR (13.13 pp 637-650; handout for ch. 13)

Valence State Electron-Pair Repulsion (VSEPR)

“classical” (electrostatic) theory of molecular geometry



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translation of book review of J.H. van't Hoff's 1874 *Sur les formules de structure dans l'espace*
by Kolbe in 1877

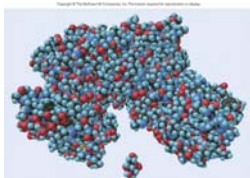


"Not long ago I expressed the view that the lack of general education and of thorough training in chemistry of quite a few professors of chemistry was one of the causes of the deterioration of chemical research in Germany... Will anyone to whom my worries may seem exaggerated please read, if he can, a recent memoir by Herr van't Hoff on *The Arrangement of Atoms in Space*, a document crammed to the hilt with outpourings of childish fantasy. This Dr. J.H. van't Hoff, employed by the Veterinary College at Utrecht, has, so it seems, not taste for accurate chemical research. He finds it more convenient to mount his Pegasus (evidently taken from the stables of the Veterinary College) and to announce how, on his daring flight to Mount Parnassus, he saw atoms arranged in space."



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a knowledge of molecular geometry is essential in biological chemistry



enzyme + sugar



[HIV-protease complex](#)

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van' Hoff had the last laugh



The Nobel Prize in Chemistry 1901

"in recognition of the extraordinary services he has rendered by the discovery of the laws of chemical dynamics and osmotic pressure in solutions"



Jacobus Henricus van't Hoff

the Netherlands

Berlin University
Berlin, Germany

b.1852

d.1911

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Basic premises of VSEPR

- ELECTRON GROUPS (non-bonding electron-pairs and covalent electron-pairs) are electron dense regions in a molecule
- these ELECTRON GROUPS will arrange themselves in space around a central atom to minimize their mutual electrostatic repulsion
- this minimum repulsion configuration determines the ELECTRONIC GEOMETRY
- the arrangement of the covalent pair regions determines MOLECULAR GEOMETRY

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electron groups

- An electron group (electron dense region) can be:
 - lone pair
 - single bond
 - multiple bond (counts as only as 1 electron group)
- The number of electron groups around the central atom is the steric number (SN)

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examples of steric number (SN)

- CH_4 SN=4
- NH_3 SN=4
- BeH_2 SN=2
- C_2H_4 SN=3
- C_2H_2 SN=2

55

the minimum repulsion "electronic" geometries are (table 13.8)

TABLE 13.8 Arrangements of Electron Pairs Around an Atom Having Minimum Repulsion

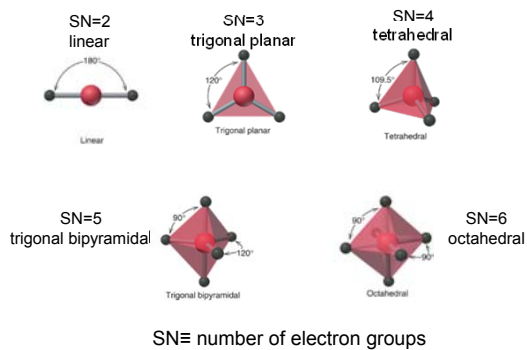
Number of Electron Pairs	Arrangement of Electron Pairs	Example
2	Linear	
3	Trigonal planar	
4	Tetrahedral	
5	Trigonal bipyramidal	
6	Octahedral	

YouTube →

[WWW Links Ch. 13 VSEPR](#) →

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the minimum repulsion "electronic" geometries are (fig. 10.2, Silb)



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SN=2: linear electronic geometry, linear molecular geometry

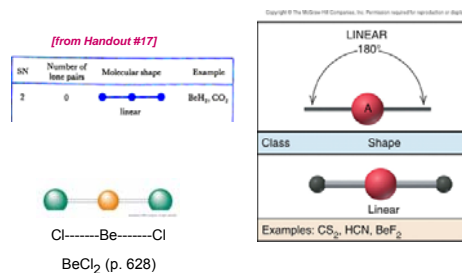


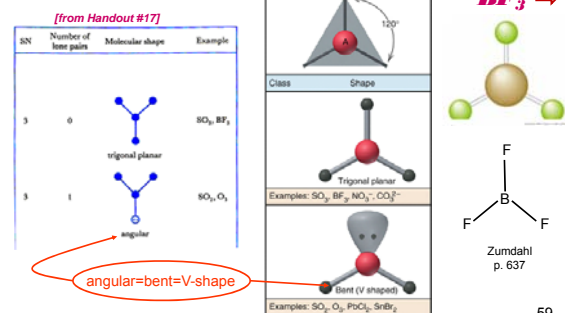
fig Silb 10.3



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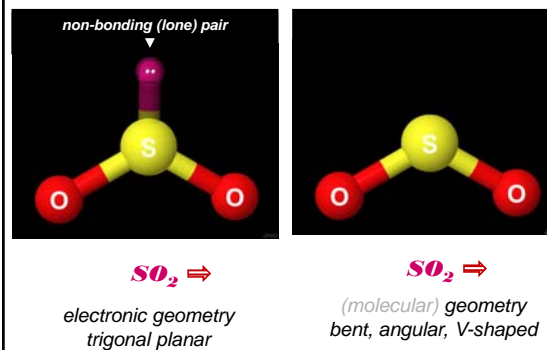
SN=3, electronic geometry is trigonal planar

examples: BF_3 SO_2



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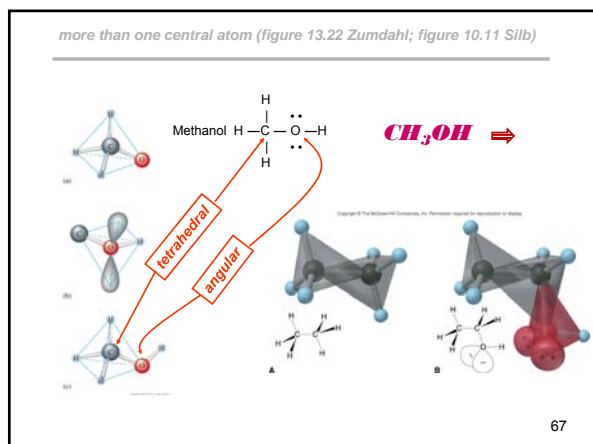
SN=3, 1 LP



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Lectures 10-11-12



Polar Molecules
Dipole Moments
and
Molecular Geometry

(Pp 600-606)

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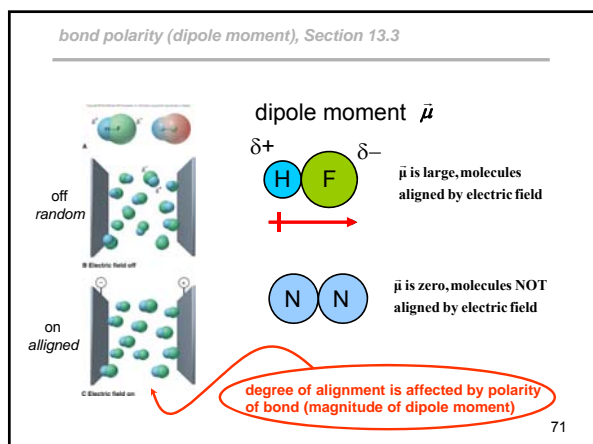
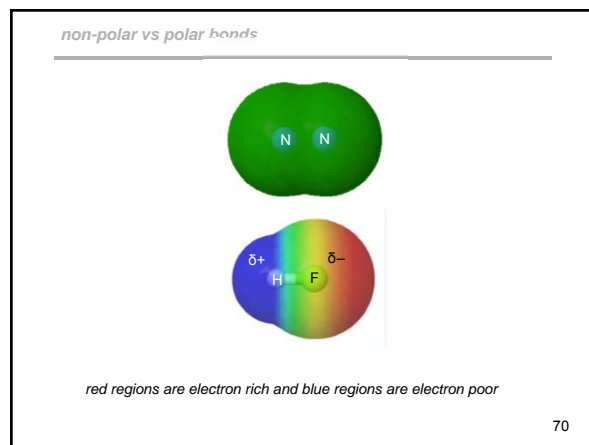
learning objectives worksheet VII (7): section IV

IV. Polyatomic dipole moments

- In a polar covalent bond the _____ electronegative atom will have a partial positive charge (δ^+) and the _____ electronegative atom will have a partial negative charge (δ^-).
- Will molecules with polar bonds always have a (non-zero) dipole moment? Explain your answer.

Modeling dipoles and electrostatic surfaces
<http://chemtube3d.com/ElectrostaticSurfacesPolar.html>

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dipole moments in polyatomic molecules

official formula for dipole moment VECTOR

$$\vec{\mu} = \sum Q_A \vec{R}_A \quad \} \text{ don't fret on this}$$

- Are there polar bonds (bond dipoles)?
- Do the bond dipoles (vectors) cancel-out or reinforce in the polyatomic molecule?

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examples

- H_2O →
- CO_2 →
- CCl_4 →
- CHCl_3

Molecular Geometry, Bond Dipoles, and Net Dipole
<http://chemtube3d.com/ElectrostaticSurfacesPolar.html>

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FINISHED For NOW !!

Short & Sweet ??

© The Electronic Reader

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END OF CHAPTER 13

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Figure 13.5, 13.7

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CCl_4 and CHCl_3

CCl_4

nada
bond dipoles cancel
no dipole moment
non-polar molecule

EN (table 13.2)

H 2.20
C 2.55
Cl 3.16

(fig. 13.3 ??)

CHCl_3

bond dipoles reinforce
dipole moment
polar molecule

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geometries where polar bonds **MAY** cancel (table 13.4)

Type	B-A-B	Cancellation of Polar Bonds	Example	Ball-and-Stick Model
Linear molecules with two identical bonds	B-A-B	← →	CO_2	
Planar molecules with three identical bonds 120 degrees apart	B B B	← ↘ ↙	SO_3	
Tetrahedral molecules with four identical bonds 109.5 degrees apart	B B B B	← ↘ ↙ ↗	CCl_4	

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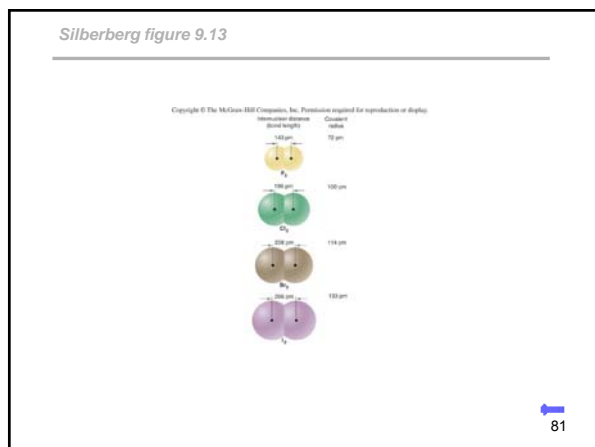
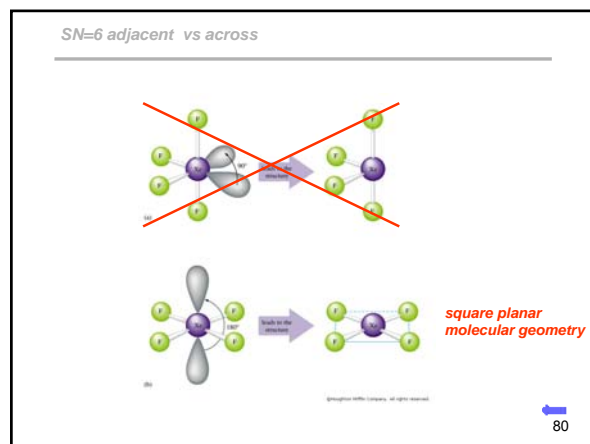
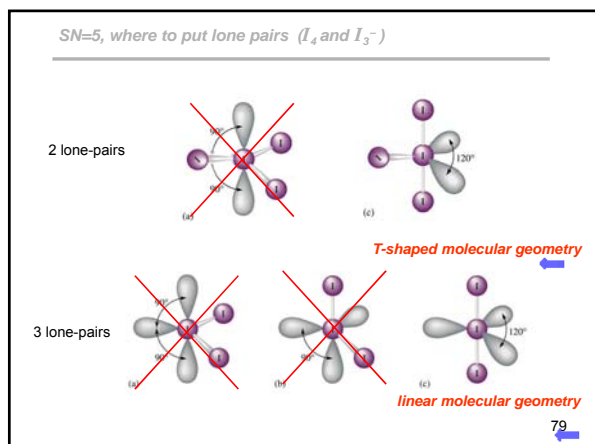


Table 13.7 Zumdahl

TABLE 13.7 Bond Lengths for Selected Bonds

Bond	Bond Type	Bond Length (Å)	Bond Energy (kJ/mol)
C—C	Single	1.54	347
C=C	Double	1.34	614
C≡C	Triple	1.20	839
C—O	Single	1.43	358
C=O	Double	1.23	745
C—N	Single	1.43	305
C=N	Double	1.38	615
C≡N	Triple	1.16	891

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Table 13.7 Zumdahl

TABLE 13.7 Bond Lengths for Selected Bonds

Bond	Bond Type	Bond Length (Å)	Bond Energy (kJ/mol)
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C=N	Double	1.38	615
C≡N	Triple	1.16	891

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Zumdahl table 13.6

TABLE 13.6 Average Bond Energies (kJ/mol)

Single Bonds			Multiple Bonds				
H—H	432	N—H	391	I—I	149	C=C	614
H—F	565	N—N	160	I—Cl	208	C≡C	839
H—Cl	427	N—F	272	I—Br	175	O=O	495
H—Br	363	N—Cl	200			C=O*	745
H—I	295	N—Br	243	S—H	347	C≡O	1072
		N—O	201	S—F	327	N=O	607
C—H	413	O—H	467	S—Cl	253	N=N	418
C—C	347	O—O	146	S—Br	218	N≡N	941
C—N	305	O—F	190	S—S	266	C=N	615
C—O	358	O—Cl	203			C≡N	891
C—F	485	O—I	234	Si—Si	340		
C—Cl	329			Si—H	393		
C—Br	276	F—F	154	Si—C	360		
C—I	240	F—Cl	433	Si—O	452		
C—S	259	F—Br	242				
		Cl—Cl	239				
		Cl—Br	218				
		Br—Br	193				

*C=O (CO₂) = 799

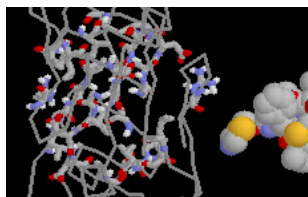
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Ritonavir inhibitor "fits into" HIV Protease



HIV protease inhibitor Ritonavir binding to the protease

<http://molvis.sdsc.edu/pe1.982/atlas/atlas.htm>

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Zumdahl Table 2.5 and 13.5, Silberberg figure 9.3

TABLE 13.5 Common Ions with Noble Gas Electron Configurations in Ionic Compounds

Group 1A	Group 2A	Group 3A	Group 4A	Group 5A	Electron Configuration
H ⁺ , Li ⁺	Be ²⁺	Al ³⁺	Ge ⁴⁺	F ⁻	[He]
Na ⁺	Mg ²⁺		Sn ⁴⁺	Cl ⁻	[Ne]
K ⁺	Ca ²⁺		Pb ⁴⁺	Br ⁻	[Ar]
Rb ⁺	Sc ³⁺		Sn ²⁺	Se ²⁻	[Kr]
Cs ⁺	Ba ²⁺		Pb ²⁺	I ⁻	[Xe]

Period	1A	2A	3A	4A	5A	6A	7A	8A
1	H	He						
2	Li	Be	B	C	N	O	F	Ne
3	Na	Mg	Al	Si	P	S	Cl	Ar

TABLE 2.5 Common Polyatomic Ions

Ion	Name	Ion	Name
NO ₂ ⁻	nitrite	CO ₃ ²⁻	carbonate
NO ₃ ⁻	nitrate	HCO ₃ ⁻	hydrogen carbonate (bicarbonate is a widely used common name)
SO ₃ ²⁻	sulfite	ClO ⁻	hypochlorite
SO ₄ ²⁻	sulfate	ClO ₂ ⁻	chlorite
HPO ₄ ²⁻	hydrogen sulfate (sulfate is a widely used common name)	ClO ₃ ⁻	chlorate
OH ⁻	hydroxide	ClO ₄ ⁻	perchlorate
CN ⁻	cyanide	C ₂ H ₃ O ₂ ⁻	acrylate
CH ₃ ⁻	methyl	MnO ₄ ⁻	permanganate
PO ₄ ³⁻	phosphate	C ₂ O ₄ ²⁻	oxalate
HPO ₄ ²⁻	hydrogen phosphate	CrO ₄ ²⁻	chromate
H ₂ PO ₄ ⁻	dihydrogen phosphate	NO ₂ ⁺	nitrosonium

KNOW:
 NH_4^+ , NO_3^- , SO_4^{2-} , HSO_4^- ,
 CN^- , OH^- , PO_4^{3-} , CO_3^{2-} ,
 HCO_3^- , $\text{C}_2\text{H}_3\text{O}_2^-$, MnO_4^-

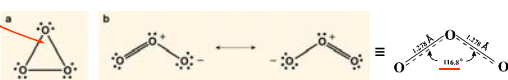
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triangular cyclic O₃

The Story of
 Roald Hoffmann
 The Ring

So now we have oxygen chemistry in the atmosphere, in the cell, in a decontamination process. But have we exhausted all of oxygen's secrets?
<http://www.americanscientist.org/issues/pub/the-story-of-o/5>

60° bond angles are "strained" (unstable);
 [discuss later in term (quantum mechanics)]



Indeed, the best calculations today confirm the metastability of this ring. Cyclic ozone lies about **130 kilojoules per mole above normal O₃** but has a barrier of no less than 95 kilojoules per mole preventing conversion to the open form.

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HW-hints Homework #4, Due 26th October

Chemistry 1B-AL
 Homework #4 (#29-#35, S8)

Required (submit via [WebAssign](#))

- 29. Zumdahl #13.15 **electronegativity**
- 30. Zumdahl #13.26 **configurations of stable ions (part c: configurations)**
- 31. Zumdahl #13.32 **LE**
- 32. Zumdahl #13.33 **LE**
- 33. Zumdahl #13.41 **common valences (oxidation states) empirical formulas**
- 34. Zumdahl #13.42 **LE**
- 35. Zumdahl #13.57 **LE**

Section

- S8. Zumdahl #13.3

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HW#4 probs 36, 39, 40

Please show problems 36, 39, and 40 with all Lewis structures for some of the same molecules and ions. Place in HW box at the end of the lecture. Show structures corresponding to the appropriate number of valence electrons for the molecule or molecular ion. **DO NOT CHARGE ON ATOMS.** They come in problem 40.

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HW#4

- 36. Zumdahl #13.54 (a) **resonance structures**
- 37. Zumdahl #13.57 **resonance structures**
- 38. Zumdahl #13.71 (a, d, and f) **formal charge (octet)**
- 39. Zumdahl #13.72 (for 13.71 a,d,f) **formal charge (non octet)**

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