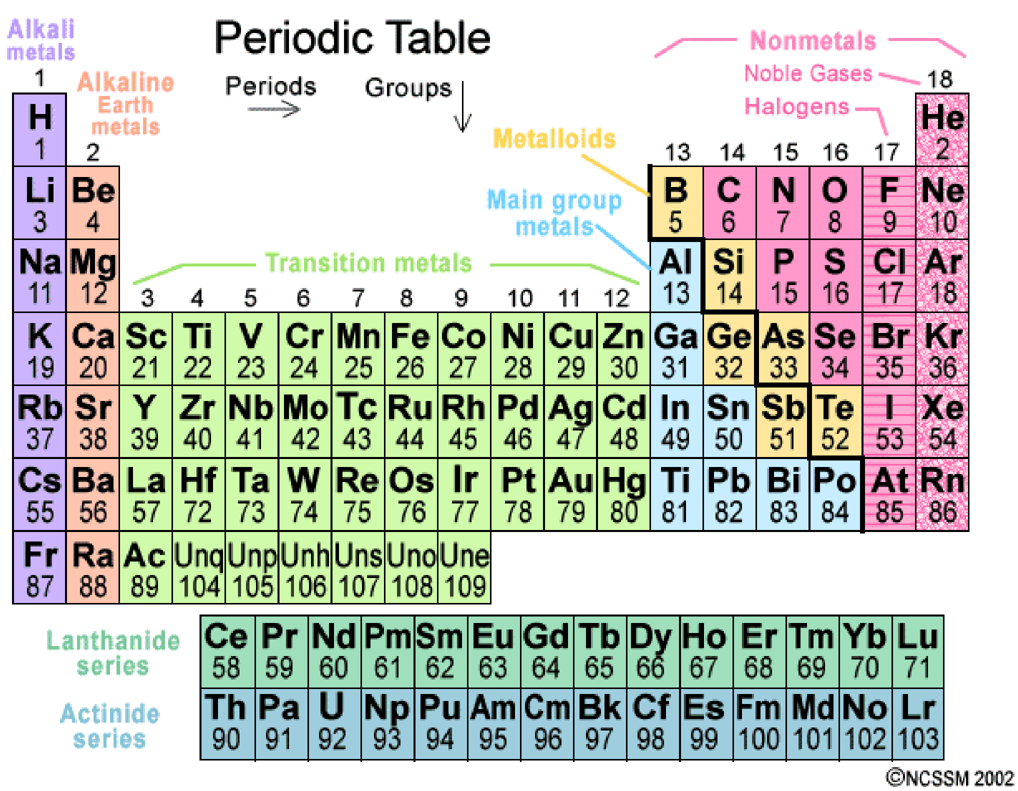
Modern Atomic Theory – Part 1

Reading:	Ch 12 sections 6 – 10	Homework:	12.6 and 12.7 questions 50, 52, 54, 56*, 58*, 60*, 62 12.8 questions 70*, 72 12.9 questions 74, 78, 80, 82*, 86*

* = ‘important’ homework question

The Electronic Structure of Atoms and Molecules

Recall: What caused Mendeleev to stack certain elements in ‘Family’ groups?



Answer:

Macroscopic properties: Elements in the same group (column) of the periodic table have similar chemical and physical properties.

e.g. All the group II elements (the alkali earths) are all metallic, form alkali solutions when mixed with water and form +2 charge cations when ionized.

Why is this? What is the underlying microscopic 'answer' that explains these facts?

Microscopic properties: Elements in the same group (column) of the periodic table have similar outer (valence) electronic configurations.

The loss /gain (ionic bonding), *or* the sharing (covalent bonding), of an atom's outer most electrons IS chemistry (recall 'old' slide*)

Chemistry is 'all about' making new materials (as described by a chemical reaction's equation) – to do this *new bonds are made* (in the products) and *old bonds are broken* (in the reactants). Bond making and breaking **ONLY** involves the outer valence electrons of atoms.

Remember Dr. Mills favorite saying……

One time British soccer icon 'Gazza' with a gyro

"Chemistry is a bit like Scottish soccer – it's basically a bunch of round things bumping into one another"

Gazza playing out his career with Glasgow Rangers

The Electronic configurations of the first 20 elements

Seven Key fact

1.

2.

3.

4.

5.

6.

7.

Important definitions:

Electron ‘dot’ symbol: Includes BOTH outer (valence) AND inner (core) electrons

Lewis symbol: Includes outer (valence) electrons ONLY

Task: Draw electron ‘dot’ *and* Lewis symbols for:

Si

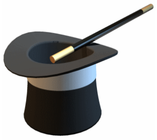
Cl

P

Add these Dot diagrams to your periodic table of electronic structure.
Complete the table for all atom types up to Ca

<u>Task</u>: Complete the following table:

Atom	Group number	Number of valence electrons	Lewis Symbol
N			
P			
O			
S			
C			
			



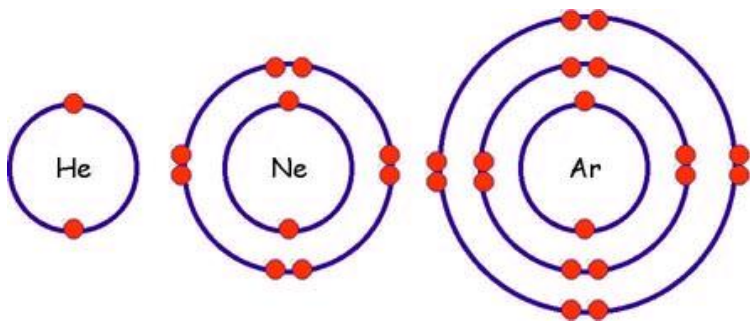
Recall that the number of valence electrons an atom has is equal to its group number – this is why elements in the same group have similar chemical properties (similar valence configurations)

The Octet Rule (Full Valence Shell rule)

ATOMS WITH FULL OUTER (VALENCE) SHELLS ARE STABLE ⇒ Atoms will lose, gain or share electrons to have an inert gas (full valence shell) configuration.

THIS IS THE 'DRIVING' FORCE BEHIND ALL CHEMICAL PROCESSES.

Inert gas (stable electron shell) configurations (**spot the error**!*)



Examples**:**

1. Ionic bonding – the formation of LiF

Recall: Ionic bonds form between atoms (metal and non-metal, which then become ions) with a large difference in electronegativity

2. Covalent bonding – the formation of F_2 (g)

Recall: Covalent bonds form between atoms (two non-metals) with little or no difference in electronegativity

Simple Lewis Structures

Overview (recall your workshop): Lewis structures are electron 'maps' of molecules, which are in turn constructed from the Lewis symbols of the molecule's component atoms.

Task: Complete the following table

Atom	Number valence electrons	Lewis Symbol	Valencey (number of bonds formed)
C			
N			
O			
Cl			
H			

The number of bonds an atom forms in a molecule

≡

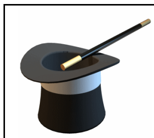
Number of UNPAIRED valence electrons (VALENCEY) it has

EZ Lewis Symbols – think of an *unpaired* valence electron as 'a hand that needs to be held' (I could not think of a more masculine analogy!). Then just have the atoms 'hold hands' (form bonds by converting unshared e^- to shared pairs of e^-) to make the required molecule's Lewis structure. **H_2O example**.

Task: Write formal Lewis symbols and 'EZ' Lewis symbols for the following atoms:

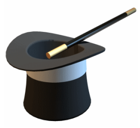
Atom	Formal Lewis Symbol*	'EZ' Lewis Symbol**
C		
N		
O		
Cl		
H		

*Always write the formal Lewis symbol on a test. **This is not to be written on any formal test!



Remember: Just have the atoms, as represented by 'EZ' Lewis symbols, 'hold hands' to make the required molecule's Lewis structure

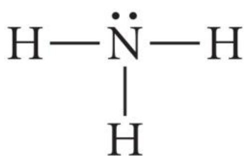
Task: Draw Lewis structures for the following molecules.



Remember: Each atom in a molecule must have as many bonds as its valencey (number of unpaired electrons). **Double or Triple bonds often arise from applying this rule**.

Note: The total number of valence electrons in a Lewis structure is simply the some of those 'owned' by each of the molecule's component atoms. **Write this information next to each of the above Lewis structures**.

Ammonia (NH_3)



Water (H_2O)

Methane (CH_4)

Phosphorus trichoride (PCl_3)

Oxygen gas (O_2)

Nitrogen Gas (N_2)

Hydrogen Fluoride (HF)

Dihydrogen monosulfide (H_2S)

Let's work on your molecular modeling lab now…

Lewis Structures for More Complex Molecules - 'The Rules'

Use the following rules to figure out the Lewis structure of ANY molecule (the above are simpler examples of the application of this 'global' set of rules)

Worked Example – Carbon Dioxide (CO_2)

1. Sum the valence electrons from all the atoms in the molecule or ion.

For anions (-ve), ADD one e^- per negative charge on the ion
For cations (+ve), SUBTRACT one e^- per positive charge on the ion

⇒ For CO_2:

2. Write the atoms on the page with the HIGHEST valencey atom in the center:

⇒ For CO_2:

3. Connect the outer atoms to the center atom with single lines(s) – these bonds (pair of shared electrons) are the minimum requirement for a molecule to exist.

4. Complete the valence shells of the 'outside' atoms to give them stable valence configurations.

5. Count up all the electrons in the structure and compare to the number required (from rule 1). Place any excess electrons on the center atom.

6. If the center atom does not have enough electrons for a complete valence shell, CONVERT ‘OUTSIDE’ LONE PAIR ELECTRONS TO DOUBLE BONDS. Remember that each outside atom’s valencey must also be obeyed.

7. Double-check the valencey of all atoms and the total number of electrons in the structure.

Task: Follow the above rules to construct Lewis structures for the following molecules and ions:

1. $CHCl_3$
2. CH_2O
3. CO_3^{2-}

Is there more than one way to write the Lewis structure of the carbonate (CO_3^{2-}) ion?

These ‘different versions’ of the Lewis structures are called *resonance structures* (class demonstration)

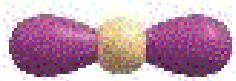
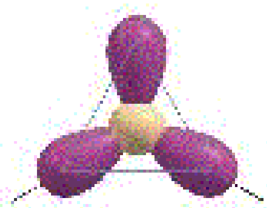
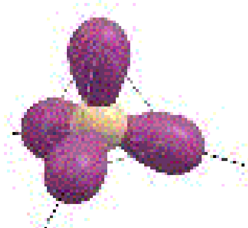
The Shape of Molecules – VSEPR Theory

The shape of any molecule in 3D can be determined by applying the Valence Shell Electron Pair Repulsion (VSEPR) Theory to a Lewis structure of the respective molecule

Electron pairs in the valence shell of a *center* atom (as drawn in a Lewis structure) *repel* one another as they have the same *negative* charge

The 3-D shape of a molecule is directly correlated to how the valence electron pairs are arranged in (3-D) in order to be as greatly separated from one another as possible

TABLE 9.1 Electron-Domain Geometries as a Function of the Number of of Electron Domains

Number of Electron Domains	Arrangement of Electron Domains	Electron-Domain Geometry	Predicted Bond Angles
2		Linear	180°
3		Trigonal planar	120°
4		Tetrahedral	109.5°

Consider each electron pair (*bonded* or *lone*) as 'clumps' of negative charge. These clumps adopt the above 3-D shapes in order to obey the VSEPR effect

<u>Examples</u>: Draw Lewis structures and determine the 3-D molecular shapes of carbon dioxide (CO_2), methanal (CH_2O) and methane (CH_4).

Molecular shape vs Electronic shape

The *molecular* (where the atoms are) and *electronic* (where the 'clumps' of electrons are) shapes of molecules are often different

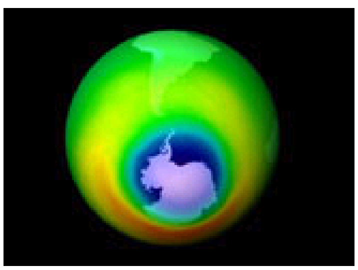
Recall: The valence electron pairs' (bonded *and* lone) determine the overall *electronic shape* of the molecule

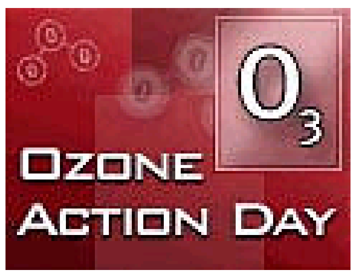
But: The positions of the molecule's atoms *relative to one another* (after the electronic shape has been fixed) determine the *molecular shape*

Examples: Draw Lewis structures and determine the 3-D molecular and electronic shapes of methane (CH_4), water (H_2O) and ammonia (NH_3).

Question of the week: Draw Lewis structure(s) for the ozone molecule (O_3) and determine its molecular shape using VSEPR theory.

Environmental Concerns

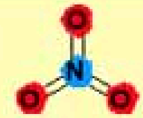
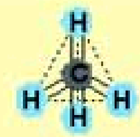
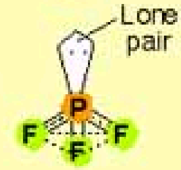
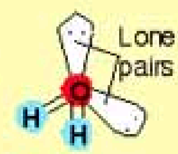

The Ozone 'hole' over Antarctica



An Ozone action day sign warning of ***excess*** O_3

Discussion: How can there simultaneously be *too much* (ozone action days) and *too little* (Antarctica's ozone 'hole') ozone in the atmosphere? Solution?

The relationship between molecular shape, electronic shape, numbers of bonding electron pairs and lone pairs of valence electrons

Electron Groups			Arrangement of Groups	Molecular Shape	Example
Total	Bonding	Lone			
2	2	0	Linear	Linear	CO_2 
3	3	0	Trigonal planar	Trigonal planar	NO_3^- 
	2	1		Bent (or angular)	O_3 
4	4	0	Tetrahedral	Tetrahedral	CH_4 
	3	1		Trigonal pyramidal	PF_3 
	2	2		Bent (or angular)	H_2O 

"Lewis"

The following question was taken from your 3rd practice midterm:

Question 3a (20 points): Draw Lewis structure(s) for the CO_3^{2-} anion, ***include all possible resonance form(s)***.

Question 3a (5 points): Use VSEPR theory to predict the electronic and molecular shape of the carbonate (CO_3^{2-}) anion.

Electronic shape:

Molecular shape: