Electrons and Bonding

Objectives

- Describe the principles and interactions responsible for atomic structure.
- Predict the charges of the single-atom ions of alkali, alkaline earth, chalcogen, and halogen elements.
- Assign an electron dot structure for a covalent molecule.
- Predict the three-dimensional structure of a covalent molecule given its electron dot structure.

Overview

Why do substances behave the way they do? How can a few dozen different chemical elements combine to form the incredible variety of materials around us? The key is *bonding*. Atoms combine with each other in specific ways to make molecules, much as sounds combine in specific ways to make meaningful words. In this activity, you will learn some of the principles by which atoms combine to form molecules.

Activity 1: Quantum numbers

For each electron in the elements listed, write the values of its four quantum numbers n (principal), l (orbital angular momentum), m_l (orbital magnetic), and m_s (spin). Identify the electron's shell and orbital type.

The quantum number n takes on whole number values 0, 1, 2, …. The orbital angular momentum quantum number l takes whole number values from 0 to n. The magnetic quantum number m_l takes integer values from –l to +l. The spin quantum number m_s can take only two values: –1/2 and +1/2. No two electrons in an atom can have the same values of all four quantum numbers. When listing quantum numbers of electrons, it is customary to start at the smallest value and increase in the smallest increment possible. Increment m_l first, then m_s, then l, and finally n. This ensures that the atom has the lowest possible energy.

Hydrogen (H)

	n	***l***	***m_l***	***m_s***	**shell**	**orbital**
1						

Helium (He)

	n	***l***	***m_l***	***m_s***	**shell**	**orbital**
1						
2						

Lithium (Li)

	n	l	m_l	m_s	**shell**	**orbital**
1						
2						
3						

Neon (Ne)

	n	l	m_l	m_s	**shell**	**orbital**
1						
2						
3						
4						
5						
6						
7						
8						
9						
10						

Sodium (Na)

	n	l	m_l	m_s	**shell**	**orbital**
1						
2						
3						
4						
5						
6						
7						
8						
9						
10						
11						

Activity 2: Valence electron configurations of atoms

Purpose

You will identify the orbitals occupied by the outer, or "valence," electrons of any neutral atom.

Materials

Periodic table

Procedure

Find the specified elements in the periodic table and use their positions in the table to determine the orbital occupancies of their valence shells.

Element	**Valence level**	**Valence electrons**	**Configuration**
Calcium	4	2	$4s^2$
Gallium			
Aluminum			
Arsenic			
Lead			
Oxygen			
Chlorine			
Sodium			
Silicon			
Sulfur			

Activity 3: Valence electron configurations of ions

Write down the valence electron configurations of the neutral atoms and ions in the table below.

Atom	Valence Configuration	Ion	Valence Configuration
Na		Na^{+}	
Mg		Mg^{2+}	
O		O^{2-}	
F		F^{-}	
K		K^{+}	
Ca		Ca^{2+}	
Cs		Cs^{+}	
Sr		Sr^{2+}	
S		S^{2-}	
I		I^{-}	

Activity 4: Covalent bonding opportunities

For each atom or ion below, determine the number of its valence electrons, portion them as evenly as possible to the four valence orbitals on a dot diagram, identify the number of unpaired electrons, and predict the number of covalent bonds the atom or ion can make.

Atom or ion	Number of Valence Electrons	Dot diagram	Unpaired electrons	Bonds possible
S		S		
H		H		
B		B		
C		C		
O		O		
O^-		O		
Cl		Cl		
Cl^-		Cl		
N		N		
P		P		
Ca^{2+}		Ca		

Activity 5: Covalent molecules

Construct dot diagrams for each individual atom and then draw the dot diagram for the diatomic covalent molecule.

Molecule	Atom diagrams		Molecule diagram
H_2	H	H	
Cl_2	Cl	Cl	
HBr	H	Br	
FCl	F	Cl	
ClI	Cl	I	

Construct the dot diagrams for each individual atom below and then draw the dot diagram for the entire polyatomic molecules.

Formula	Atom diagrams			Molecule diagram
CH_4	C	H		
CCl_4	C	Cl		
NH_3	N	H		
CH_2Cl_2	C	H	Cl	
NH_2Cl	N	H	Cl	
BF_3	B	F		

Activity 6: Multiple Centers

Draw legal dot structures corresponding to the molecular formulas given below. Some of the formulas may be satisfied by more than one structure.

CH_4O

C_2H_6

NH_3O

C_2H_7N (two structures)

$C_3H_8O_3$ (make a structure in which no two oxygen atoms are attached to each other or to the same carbon atom)

Activity 7: Double and triple bonds

Begin by drawing structures with single bonds between atoms and then complete the atoms' octets by drawing additional bonds between adjacent atoms with unpaired electrons. Hints about the structures are given for some of the cases; you will need to figure out a structure in which bonding is satisfied for the other cases. Do not draw any cyclic molecules! (Cyclic molecules can exist, but multiple-bonded molecules are the point of this activity.) It may help to use tiles and beans to keep track of all the electrons.

C_2H_4 (two hydrogens attach to each carbon)

CH_2O (If you can't satisfy the atoms' octets, try moving an H atom.)

CH_2O_2 (one hydrogen attaches to the carbon, the other to an oxygen, oxygens don't attach to each other)

$COCl_2$

$C_2H_5NO_2$ (there are several possible structures)

Activity 8: Expanded valence shells

This worksheet will step you through making dot structures of compounds containing expanded-valence atoms. The whole process boils down to breaking a non-bonding electron pair into two unpaired electrons by promoting one electron from the filled *s* or *p* orbital into an empty *d* orbital.

For each element indicated in the compounds below,

1. Determine how many bonds the indicated atom needs to have in the molecule so that the other atoms have the number of bonds they need.

2. Determine how many valence electrons the neutral atom has from its position in the periodic table.

3. Make the atom's dot structure by placing dots around the element symbol until the number of dots equals the number of valence electrons.

4. Draw an orbital diagram for the atom by marking the circles representing the *s* and *p* orbitals, one mark per electron.

5. Determine the number of covalent bonds the atom wants to make with other atoms: this is the number of single dots around the element symbol and the number of orbital circles containing exactly one mark.

6. Count the number of non-bonding pairs around the atom: this is the number of pairs of dots around the element symbol, and the number of orbital circles with "×" marked in them.

7. Now there is a decision: Is it necessary to expand the element's valence shell? To decide, look at the number of bonds needed from step 1. If this number is larger than the number of bonds the central atom wants to make in step 5 above, expanding the valence shell is necessary.

8. To allow the atom to make more bonds: break up one or more of the atom's non-bonding pairs by promoting one of its two electrons to the lowest available *d* valence orbital. Breaking up one non-bonding pair allows the atom to form two additional bonds. Make a new orbital diagram to show the new electron configuration.

9. Determine the number of covalent bonds the atom wants to make with other atoms: this is the number of orbital circles in 8 containing exactly one mark.

10. Count the number of non-bonding pairs around the atom: this is the number of orbital circles in 8 with "×" marked in them.

11. Draw the dot structure for the central atom that corresponds to the new orbital diagram. This will have a pair of dots for every "×"-marked circle in the orbital diagram, and an unpaired dot for every "\"-marked circle in the orbital diagram.

12. Draw the dot structure for the whole molecule. All atoms should have the proper number of bonds and non-bonding electron pairs.

S in SO_2:

1. Bonds needed: __	2. _____ valence electrons	3. Diagram:
4. ○ ○○○	5. ______ bonds	6. ____ non-bonding pairs. 7. Expand? yes no
8. ○ ○○○ ○○○○○	9. ______ bonds	10. ______ non-bonding pairs.
11. Central atom:	12. Molecule:	

P in PF_5:

1. Bonds needed: __	2. _____ valence electrons	3. Diagram:
4. ○ ○○○	5. ______ bonds	6. ____ non-bonding pairs. 7. Expand? yes no
8. ○ ○○○ ○○○○○	9. ______ bonds	10. ______ non-bonding pairs.
11. Central atom:	12. Molecule:	

S in SF_4:

1. Bonds needed: __	2. _____ valence electrons	3. Diagram:
4. ○ ○○○	5. ______ bonds	6. ____ non-bonding pairs. 7. Expand? yes no
8. ○ ○○○ ○○○○○	9. ______ bonds	10. ______ non-bonding pairs.
11. Central atom:	12. Molecule:	

Cl in ClF_3:

1. Bonds needed: __	2. _____ valence electrons	3. Diagram:
4. ○ ○○○	5. ______ bonds	6. ____ non-bonding pairs. 7. Expand? yes no
8. ○ ○○○ ○○○○○	9. ______ bonds	10. ______ non-bonding pairs.
11.	12.	

P in $POCl_3$:

1. Bonds needed: __	2. _____ valence electrons	3. Diagram:
4. ○ ○○○	5. ______ bonds	6. ____ non-bonding pairs. 7. Expand? yes no
8. ○ ○○○ ○○○○○	9. ______ bonds	10. ______ non-bonding pairs.
11. Central atom:	12. Molecule:	

Kr in KrF_2:

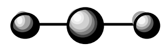
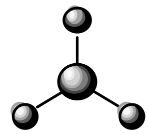
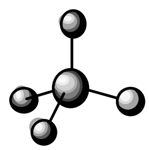
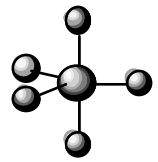
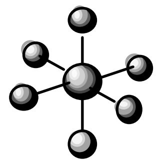
1. Bonds needed: __	2. _____ valence electrons	3. Diagram:
4. ○ ○○○	5. ______ bonds	6. ____ non-bonding pairs. 7. Expand? yes no
8. ○ ○○○ ○○○○○	9. ______ bonds	10. ______ non-bonding pairs.
11. Central atom:	12. Molecule:	

Valence Shell Electron Pair Repulsion (VSEPR) Theory

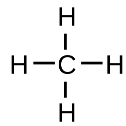
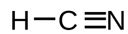
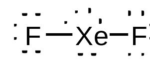
VSEPR explains how the atoms and nonbonding electron pairs attached to an atom are arranged. The different attachments repel each other, so the best arrangement is the one that keeps them as far apart as possible. The particular pattern of an arrangement depends on how many attachments there are around the central atom.

The table below shows the best arrangements for 2–6 attachments.

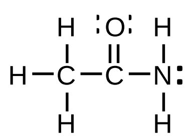
Arrangements of "Things" Attached to a Central Atom

Number of Substituents	Name of Shape	Picture of Shape
2	linear	
3	trigonal planar	
4	tetrahedral	
5	trigonal bipyramidal	
6	octahedral	

To determine which shape the attachments around an atom take, you must count the number of "things" that are attached to the atom. Each atom and each non-bonding electron pair counts as a "thing." These numbers can be found by looking at the molecule's dot structure. Some examples are shown in the table below.

dot structure			
number of atoms attached to the central atom	4	2	2
number of non-bonding electron pairs attached to the central atom	0	0	3
total "things"	4	2	5
arrangement	tetrahedral	linear	trigonal bipyramidal

If a molecule contains more than one "central" atom (an atom with more than one other atom attached to it), it is necessary to determine the arrangements of "things" around *all* of the central atoms. So, for example, the atoms in the molecule



can be predicted to arrange themselves as shown below.

central atom	left C	right C	N
atoms	4	3	3
pairs	0	0	1
total "things"	4	3	4
arrangement	tetrahedral	trigonal planar	tetrahedral

Activity 9. Shapes of covalent molecules

For each compound below,

(a) Construct the dot structure.

(b) Count the number of atoms and non-bonding pairs attached to each vertex (with more than one other atom bonded to it) atom in the molecule.

(c) For each vertex atom in the molecule, add together the two numbers from b. This is its number of substituents.

(d) From the number of substituents around each vertex atom from c, identify its base shape.

(e) Draw the molecule, showing its shape.

1. $C_4H_{10}O$ (many possible structures — choose one that is straight, no branches)

(a)
(b) atoms: pairs:
(c)
(d)
(e)

2. SF_6

(a)
(b) atoms: pairs:
(c)
(d)
(e)

3. C_5H_{12} (many possible structures — choose one)

(a)	
(b)	atoms: pairs:
(c)	
(d)	
(e)	

4. XeF_2

(a)	
(b)	atoms: pairs:
(c)	
(d)	
(e)	

5. SbF_5

(a)	
(b)	atoms: pairs:
(c)	
(d)	
(e)	

6. C_3H_9N (many possible structures — choose one)

(a)	
(b)	atoms: pairs:
(c)	
(d)	
(e)	

7. C_2H_2

(a)	
(b)	atoms: pairs:
(c)	
(d)	
(e)	

8. XeO_2

(a)	
(b)	atoms: pairs:
(c)	
(d)	
(e)	

9. $H_2C{=}O$

(a)	
(b)	atoms: pairs:
(c)	
(d)	
(e)	

10. N_2H_4

(a)	
(b)	atoms: pairs:
(c)	
(d)	
(e)	