CHEMISTRY

Chapter 7 CHEMICAL BONDING AND MOLECULAR GEOMETRY

Kevin Kolack, Ph.D.
The Cooper Union

HW problems: 5, 8, 13, 17, 21, 25, 30, 35, 45, 47, 52, 58, 65, 70, 75, 81, 89, 93, 99, 105, 116

CH. 7 OUTLINE

7.3 Lewis Symbols

7.1 Ionic Bonding

7.2 Covalent Bonding

7.3 Lewis Structures

7.4 Formal Charges and Resonance

7.5 Strengths of Ionic and Covalent Bonds

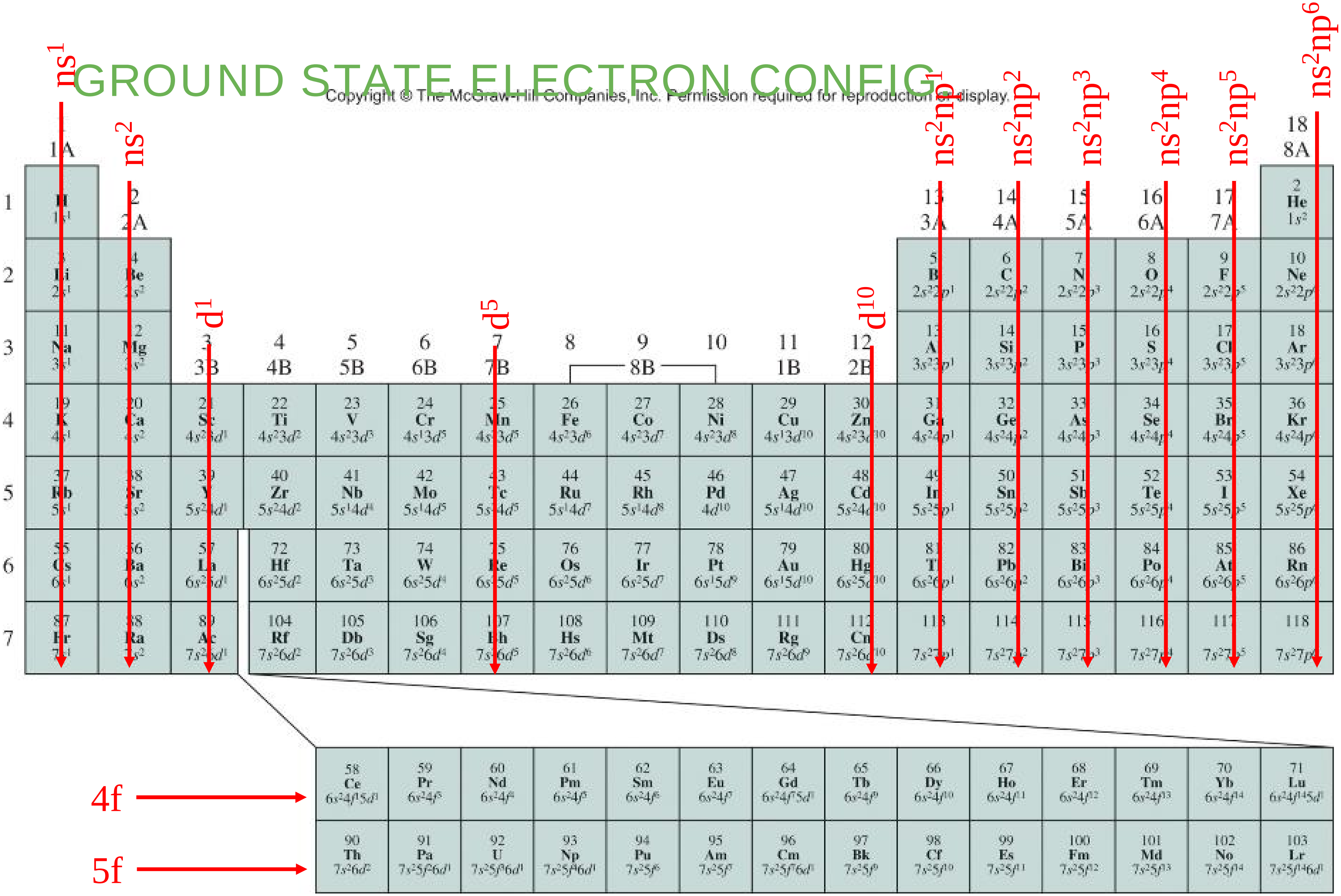
7.6 Molecular Structure and Polarity

VALENCE ELECTRONS

- The outer shell electrons of an atom. The valence electrons are the electrons that participate in chemical bonding.

Group	e^- configuration	# of valence e^-
1A	ns^1	1
2A	ns^2	2
3A	ns^2np^1	3
4A	ns^2np^2	4
5A	ns^2np^3	5
6A	ns^2np^4	6
7A	ns^2np^5	7

GROUND STATE ELECTRON CONFIG.



e^- CONFIGS OF CATIONS AND ANIONS

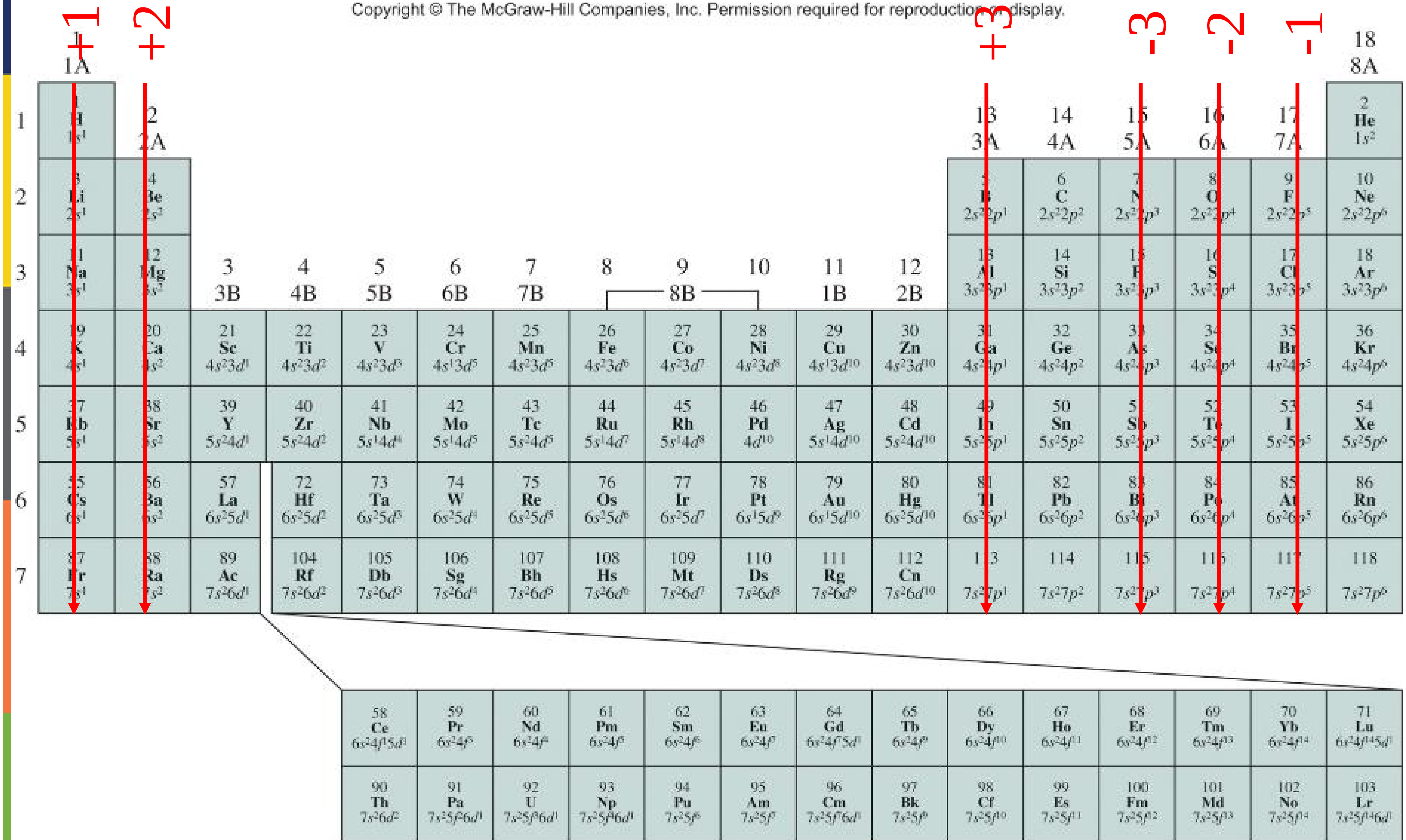
Na [Ne]$3s^1$	Na^+ [Ne]
Ca [Ar]$4s^2$	Ca^{2+} [Ar]
Al [Ne]$3s^23p^1$	Al^{3+} [Ne]

Metals lose electrons so that the cation has a noble gas e^- configuration.

Nonmetals gain electrons so that the anion has a noble gas e^- configuration.

H $1s^1$	H^- $1s^2$ or [He]
F $1s^22s^22p^5$	F^- $1s^22s^22p^6$ or [Ne]
O $1s^22s^22p^4$	O^{2-} $1s^22s^22p^6$ or [Ne]
N $1s^22s^22p^3$	N^{3-} $1s^22s^22p^6$ or [Ne]

CHARGES OF CATIONS AND ANIONS



WHY?

ISOELECTRONIC: having the same number of electrons

Being isoelectronic with a noble gas imparts added stability to a cation or anion

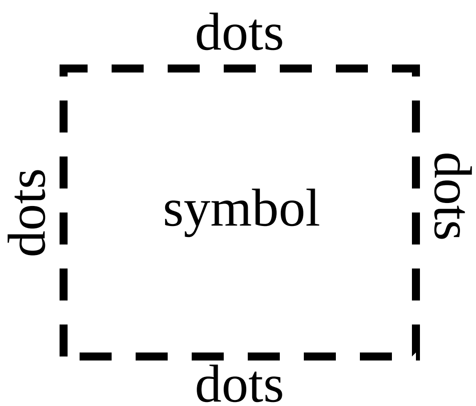
Na^+: [Ne] Al^{3+}: [Ne] F^-: $1s^22s^22p^6$ or [Ne]

O^{2-}: $1s^22s^22p^6$ or [Ne] N^{3-}: $1s^22s^22p^6$ or [Ne]

Na^+, Al^{3+}, F^-, O^{2-}, and N^{3-} are all ***isoelectronic*** with Ne

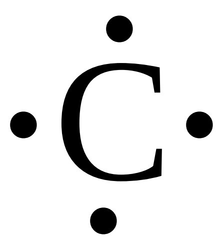
LEWIS DOT SYMBOLS

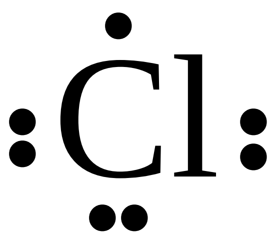
- Lewis symbol (Lewis structure) - a way to represent atoms using the element symbol and valence electrons as dots
- As only valence electrons participate in bonding, this makes it much easier to work with the octet rule
- The number of dots used corresponds directly to the number of valence electrons located in the outermost shell of the atoms of the element



LEWIS SYMBOLS (CONT'D)

- The four sides around the atomic symbol can each have two dots for a maximum of eight (octet).
- Drawing Lewis symbols
  - Place one dot on each side until there are four dots around the symbol
  - Now add a second dot to each side in turn
  - The number of valence electrons limits the number of dots placed
  - Each unpaired dot (unpaired electron of the valence shell) is available to form a chemical bond
  - Ex: carbon and chlorine





CH. 7 OUTLINE

7.3 Lewis Symbols

7.1 Ionic Bonding

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IONIC BONDING

- The electrostatic force that holds ions together in an ionic compound.
- Electrons are TRANSFERRED from element that becomes cation to element that becomes anion, maintaining ELECTRONEUTRALITY.

$$\cdot\text{Li} + :\underset{\cdot\cdot}{\overset{\cdot\cdot}{\text{F}}}\cdot \longrightarrow \text{Li}^{+}:\underset{\cdot\cdot}{\overset{\cdot\cdot}{\text{F}}}:^{-}$$

$1s^22s^1$ $\quad$ $1s^22s^22p^5$ $\quad$ $1s^2$ $\quad$ $1s^22s^22p^6$

[He] $\quad$ [Ne]

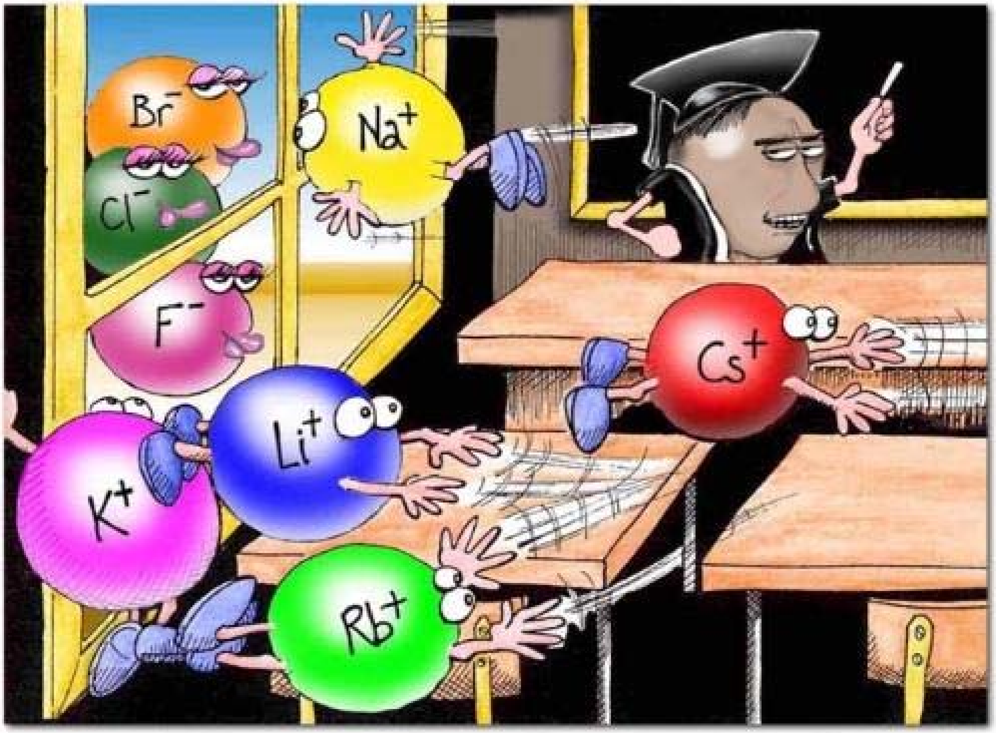
$$\cdot\text{Li} \longrightarrow \text{Li}^{+} + e^{-}$$

$$e^{-} + :\underset{\cdot\cdot}{\overset{\cdot\cdot}{\text{F}}}\cdot \longrightarrow :\underset{\cdot\cdot}{\overset{\cdot\cdot}{\text{F}}}:^{-}$$

$$\text{Li} + :\underset{\cdot\cdot}{\overset{\cdot\cdot}{\text{F}}}\cdot \longrightarrow \text{Li}^{+}:\underset{\cdot\cdot}{\overset{\cdot\cdot}{\text{F}}}:^{-}$$

IONIC BONDING

- Remember: representative (main group) elements form ions that obey the octet rule
- Ions of opposite charge attract each other resulting in an ionic bond
- Electrons are lost by a metal and they are gained by a nonmetal
  - Each atom achieves a noble gas configuration
  - 2 ions are formed; a cation and anion, which are attracted to each other



"Perhaps one of you gentlemen would mind telling me just what it is outside the window that you all find so attractive..?"

Nick Kim http://www.lab-initio.com/screen_res/nz086.jpg

IONIC BONDING EXAMPLE

Consider the formation of NaCl

Na + Cl → NaCl

Sodium has a low ionization energy; it readily loses an electron

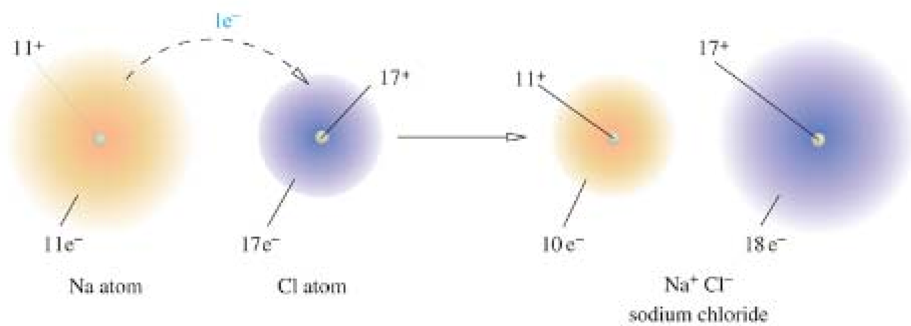
$$Na\cdot \rightarrow Na^+ + e^-$$

When sodium loses the electron, it attains a [Ne] configuration

Chlorine has a high electron affinity

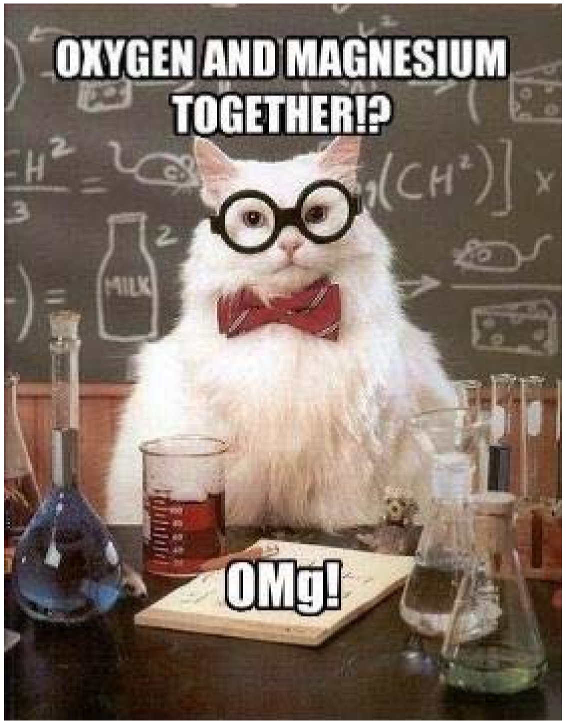
When chlorine gains an electron, it attains an [Ar] configuration

$$:\overset{..}{\underset{..}{Cl}}\cdot + e^- \rightarrow \left[:\overset{..}{\underset{..}{Cl}}:\right]^-$$



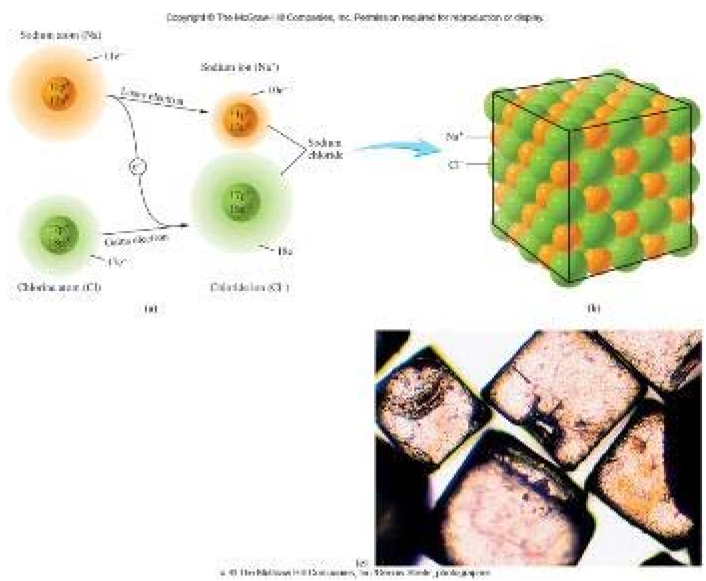
FEATURES OF IONIC BONDING

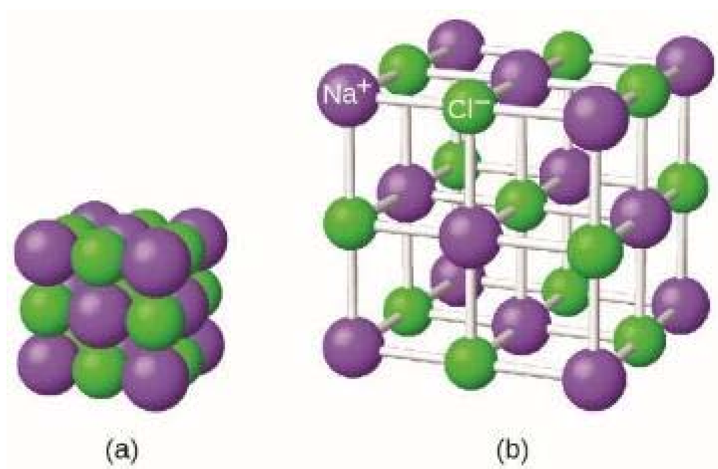
- Metals tend to form cations because they have low IE and low EA
- Nonmetals tend to form anions because they have high IE and high EA
- Ions are formed by the transfer of electrons
- The oppositely charged ions formed are held together by an electrostatic force
- Reactions between metals and nonmetals tend to form ionic compounds



ION ARRANGEMENT IN A CRYSTAL

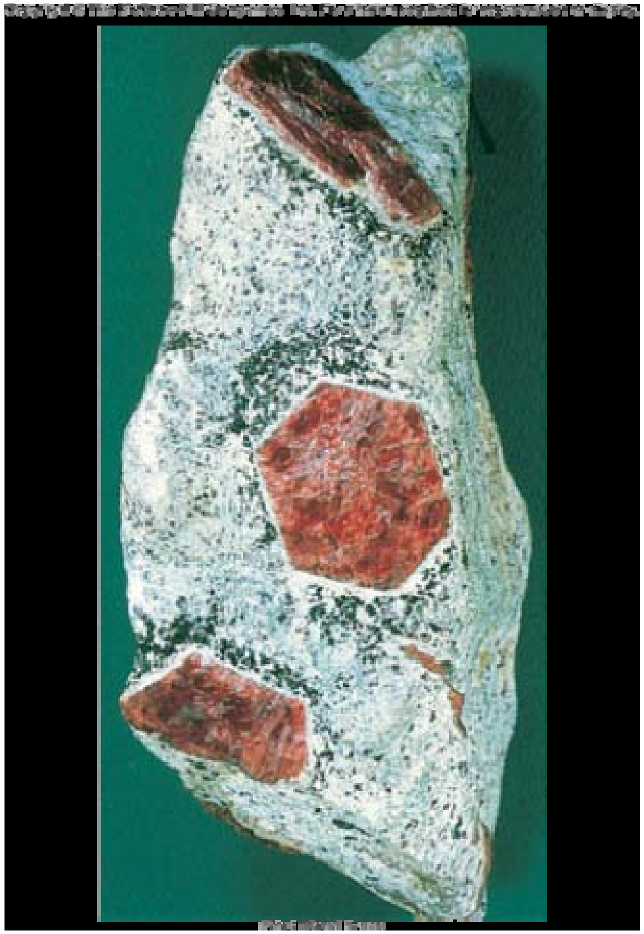
- As a sodium atom loses one electron, it becomes a smaller sodium ion
- When a chlorine atom gains that electron, it becomes a larger chloride ion
- Attraction of the Na cation with the Cl anion forms NaCl ion pairs that aggregate into a crystal, an <u>infinite array</u> of alternating Na and Cl ions in 3 dimensions





EXAMPLE

Use Lewis dot symbols to show the formation of aluminum oxide (Al_2O_3), aka the mineral corundum.



Corundum (Al_2O_3)

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COVALENT BONDING – AN INTRODUCTION

- Let's look at the formation of H_2:
- $H + H \rightarrow H_2$
- Each hydrogen has one electron in its valance shell
- If it were an ionic bond it would look like this:

$$\boxed{H\cdot + H\cdot \rightarrow H^{+} + [H:]^{-}}$$

- However, both hydrogen atoms have an <u>equal</u> tendency to gain or lose electrons
- Electron transfer from one H to another will not occur under normal conditions...

COVALENT BONDING (CONT'D)

Instead, each atom attains a noble gas configuration by <u>sharing</u> electrons

$$H\cdot + \cdot H \rightarrow H:H$$

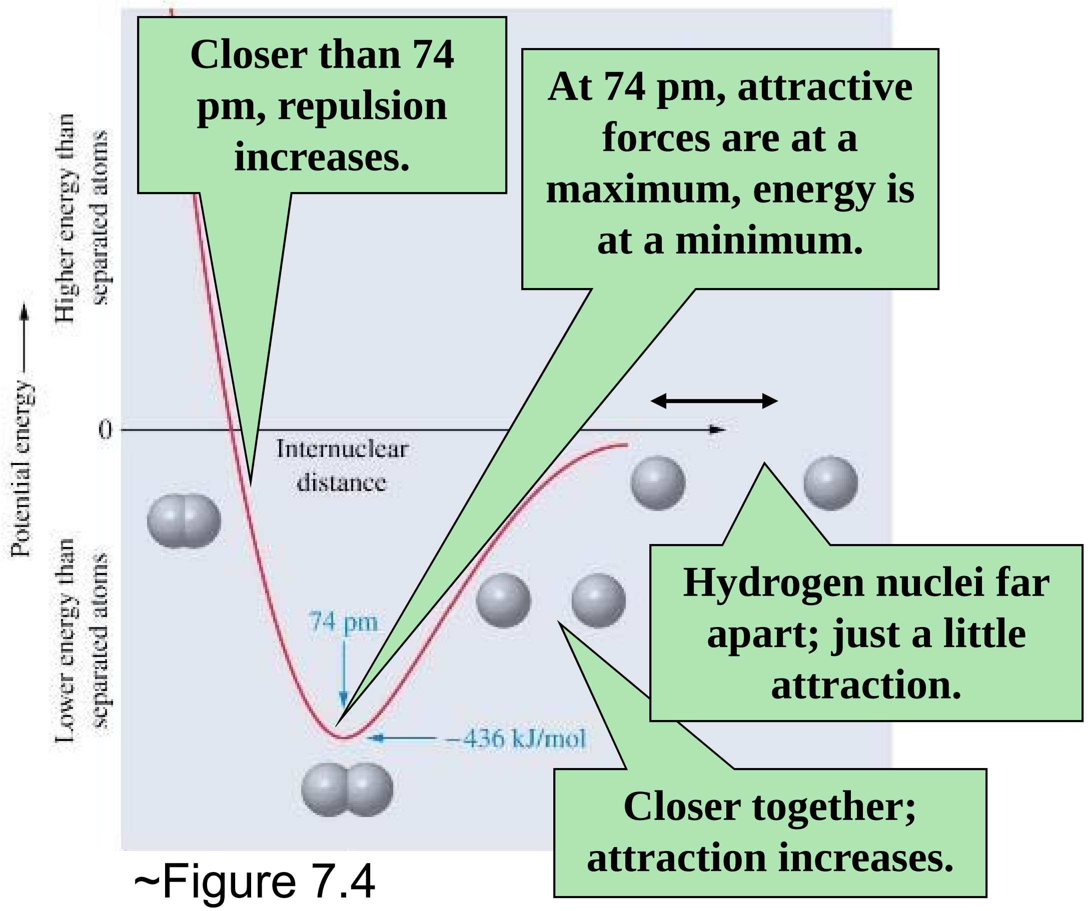
Each hydrogen atom now has two electrons around it and has attained a [He] configuration

The shared electron pair is called a covalent bond

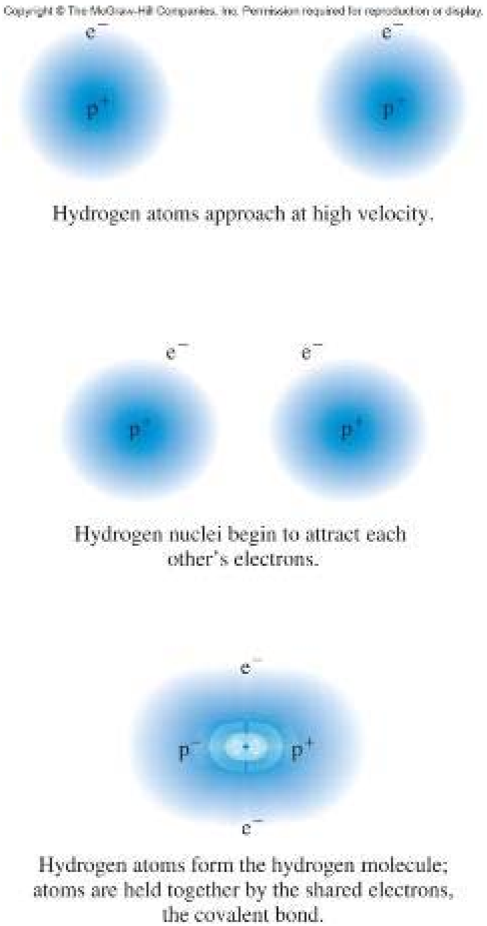
BOND LENGTH

Sharing (covalent bonding) is due to overlap of orbitals

Change in potential energy of two hydrogen atoms as a function of their distance of separation



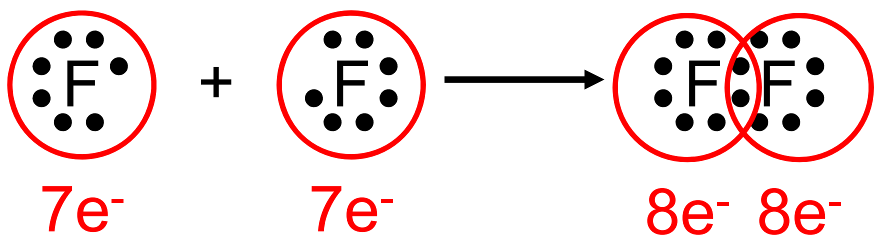
~Figure 7.4



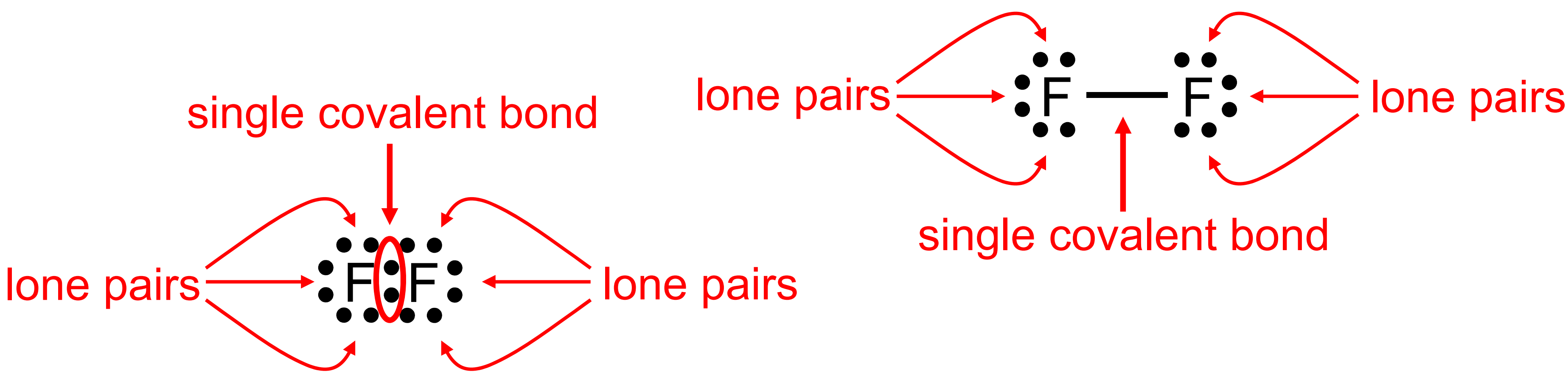
COVALENT BONDING DEFINED

- A chemical bond in which two or more electrons are shared by two atoms.

Why should two atoms share electrons?

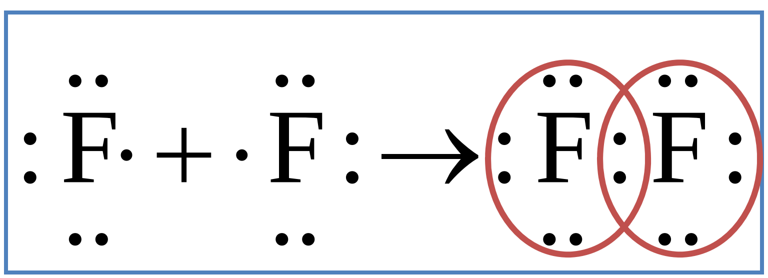


Lewis structure of F_2



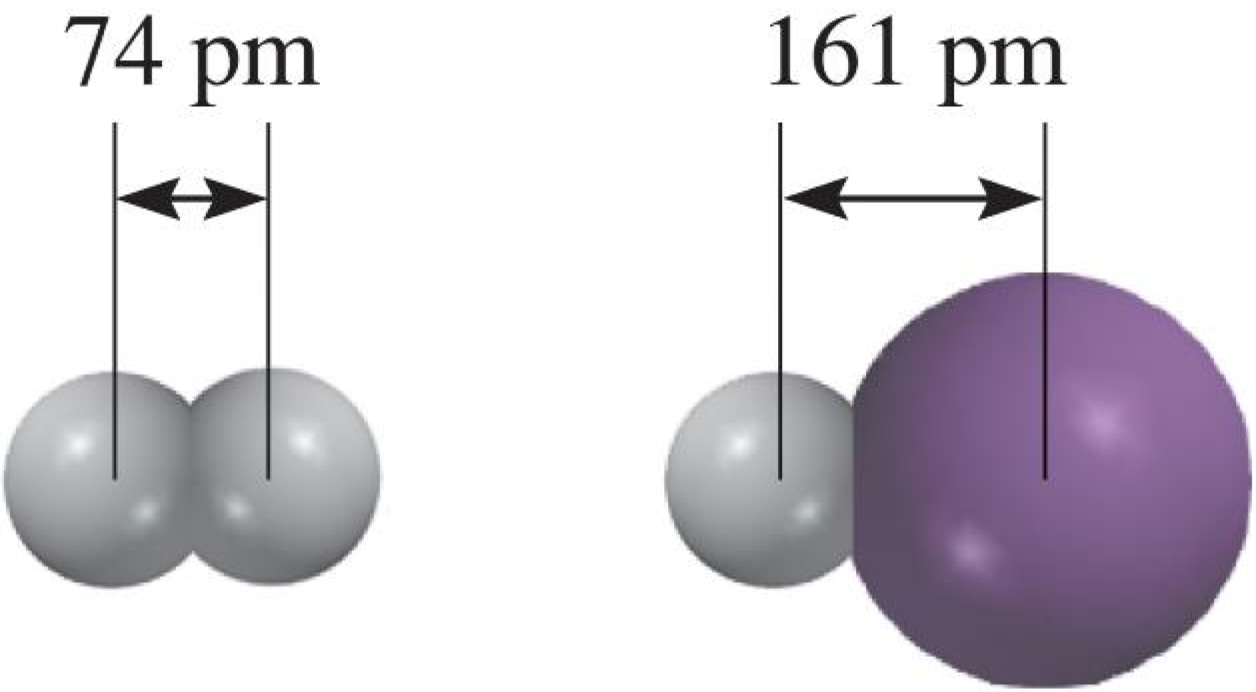
FEATURES OF COVALENT BONDS

- Covalent bonds form between atoms with similar tendencies to gain or lose electrons
  - ie, near each other on the periodic table
- Compounds containing covalent bonds are called “covalent compounds” or “molecules”
- The diatomic elements have *completely* covalent bonds (totally equal sharing)
  - H_2, N_2, O_2, F_2, Cl_2, Br_2, I_2



Each fluorine is surrounded by 8 electrons…a [Ne] configuration

BOND LENGTH



H_2 HI

Average Bond Lengths of Some Common Single, Double, and Triple Bonds

Bond Type	Bond Length (pm)
C—H	107
C—O	143
C=O	121
C—C	154
C=C	133
C≡C	120
C—N	143
C=N	138
C≡N	116
N—O	136
N=O	122
O—H	96

Bond Lengths

triple bond < double bond < single bond

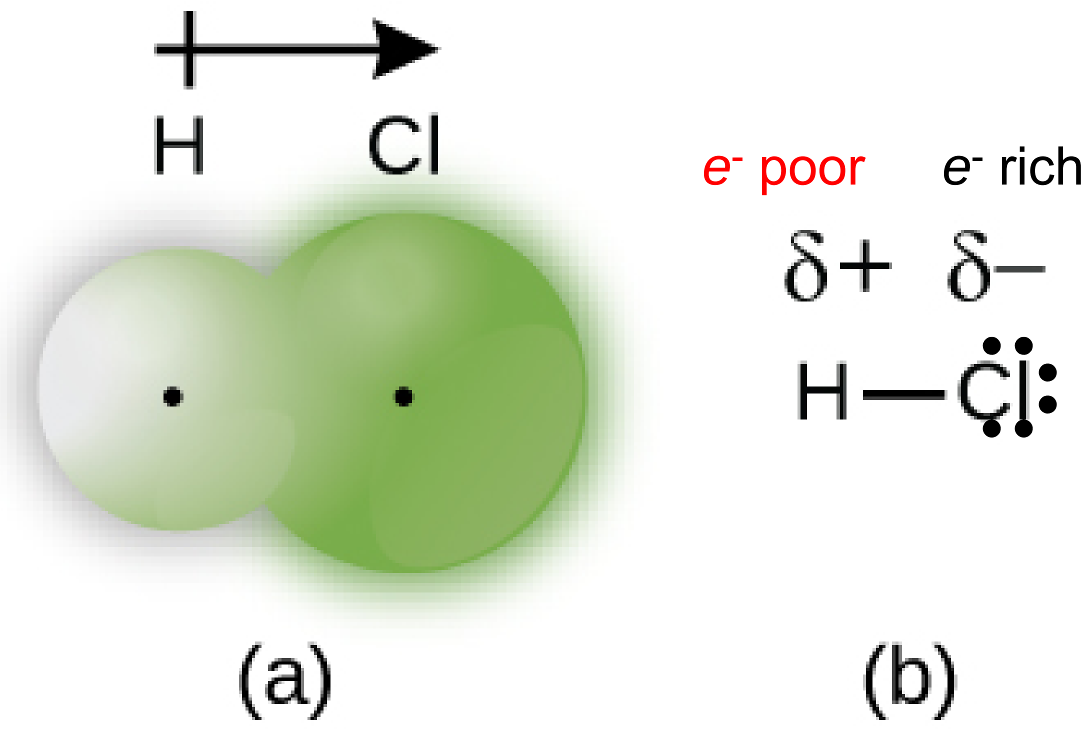
IONIC VS. COVALENT PROPERTIES

Property	NaCl	CCl_4
Appearance	White solid	Colorless liquid
Melting point (°C)	801	−23
Molar heat of fusion* (kJ/mol)	30.2	2.5
Boiling point (°C)	1413	76.5
Molar heat of vaporization* (kJ/mol)	600	30
Density (g/cm^3)	2.17	1.59
Solubility in water	High	Very low
Electrical conductivity		
Solid	Poor	Poor
Liquid	Good	Poor

*Molar heat of fusion and molar heat of vaporization are the amounts of heat needed to melt 1 mole of the solid and to vaporize 1 mole of the liquid, respectively.

POLAR COVALENT BONDING

- A polar covalent bond or polar bond is a covalent bond with greater electron density around one of the two atoms



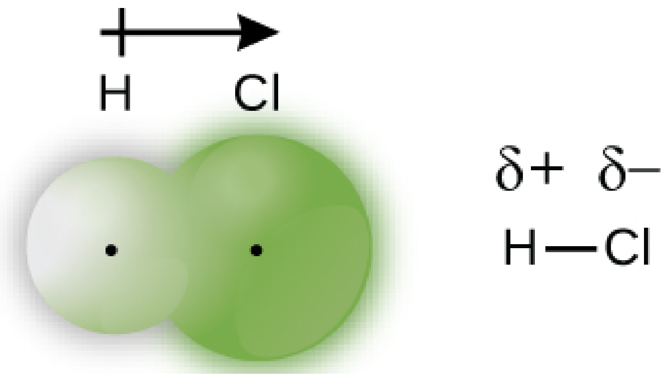
ELECTRONEGATIVITY

- The ability of an atom to attract the electrons in a chemical bond. Attraction for shared electrons.
- Similar to electron affinity, but NOT the same

Electron affinity - measurable (Cl is highest)

$$X(g) + e^- \longrightarrow X^-(g)$$

Electronegativity - relative (F is highest)



(a) (b)

PAULING ELECTRONEGATIVITY VALUES

- Increases up to the right
  - (F is the most electronegative element on the periodic table)

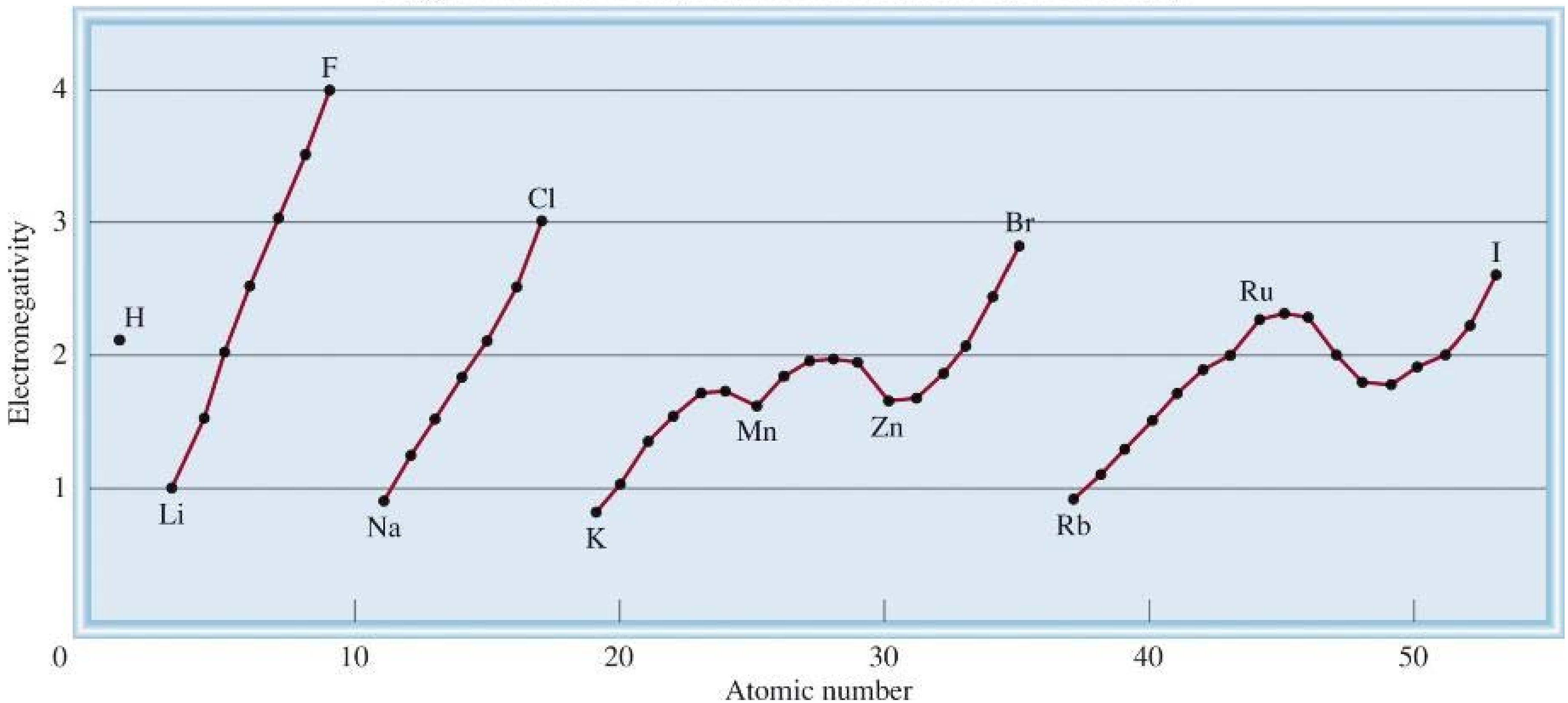
Increasing electronegativity →

Decreasing electronegativity ↓

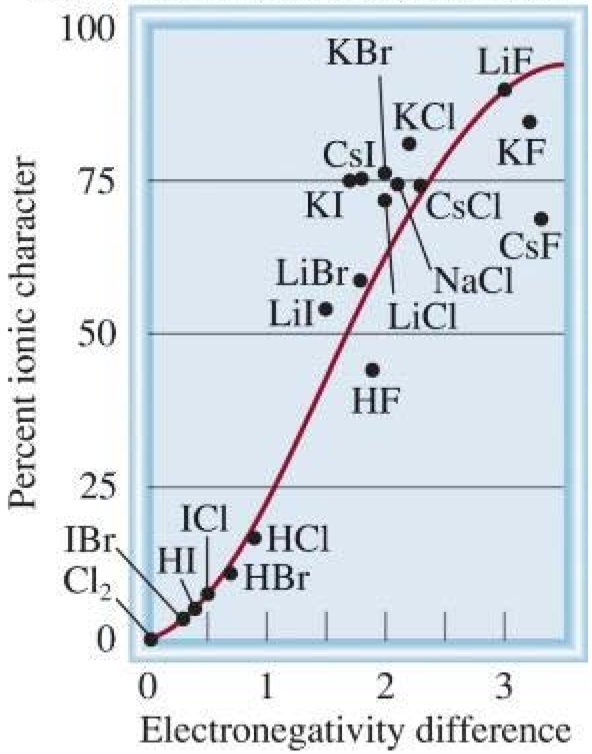
			H 2.1													
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.9	Ni 1.9	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5
Cs 0.7	Ba 0.9	La–Lu 1.0–1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.9	Bi 1.9	Po 2.0	At 2.2
Fr 0.7	Ra 0.9	Ac 1.1	Th 1.3	Pa 1.4	U 1.4	Np–No 1.4–1.3										

Linus Pauling (1901–1994) made many important contributions to the field of chemistry. He was also a prominent activist, publicizing issues related to health and nuclear weapons.

PERIODIC VARIATION IN EN VALUES

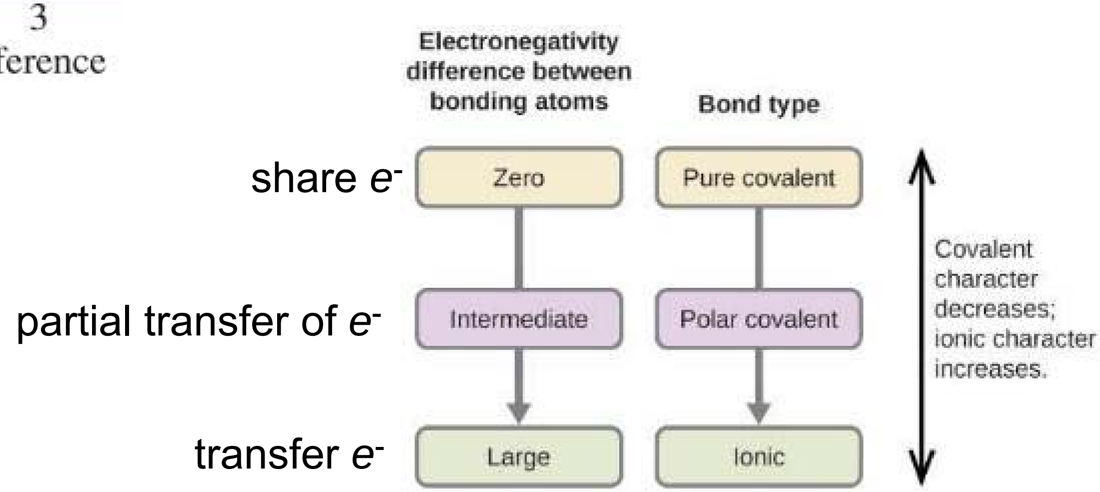


ELECTRONEGATIVITY DIFFERENCES



Difference*	Bond Type
≥ "1.8"	Ionic
"0.4" < and < "1.8"	Polar Covalent
< "0.4"	Covalent

*(These values vary from book to book.)



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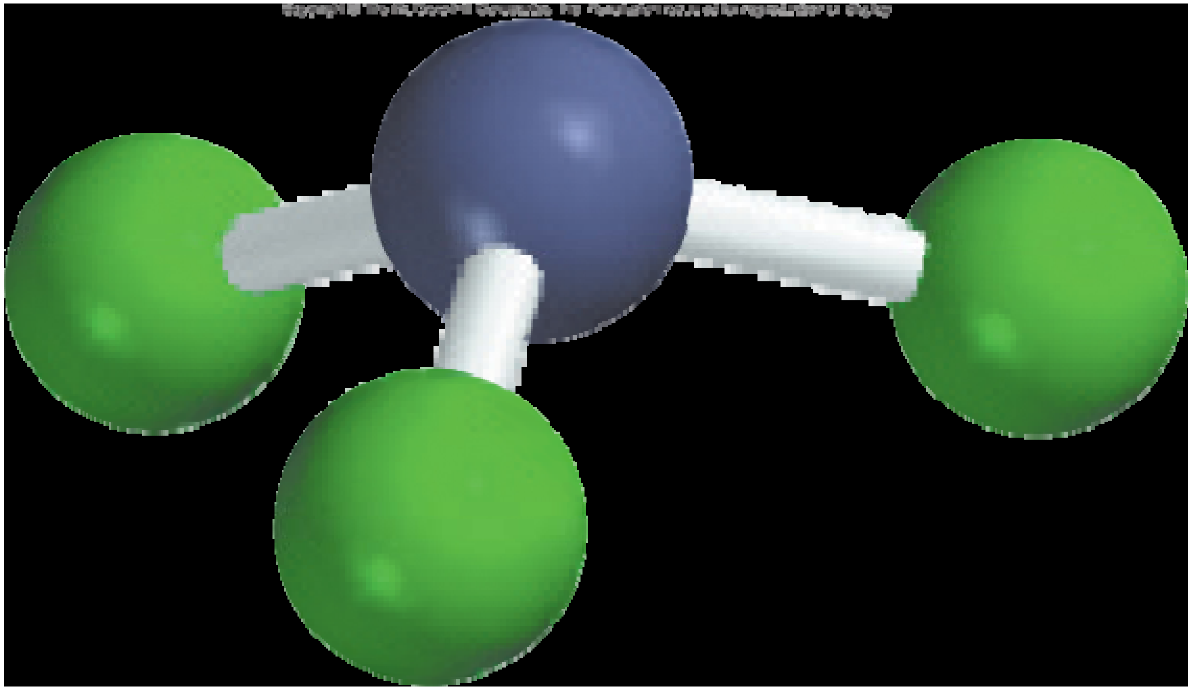
WRITING LEWIS STRUCTURES

- (I do not like your book method- surprise!)

1. Go for symmetry
   - (usually, least electronegative element at the center)
2. Treat every element like a 4-sided box and add dots
3. Connect the dots
   - Go for octets
     a) (there MUST be an octet for C, N, O, F)
     b) (3p and larger elements can have more than 8)
     c) (B and other small elements may have fewer than 8)
     d) (H and He get a "duet")
4. Clean up

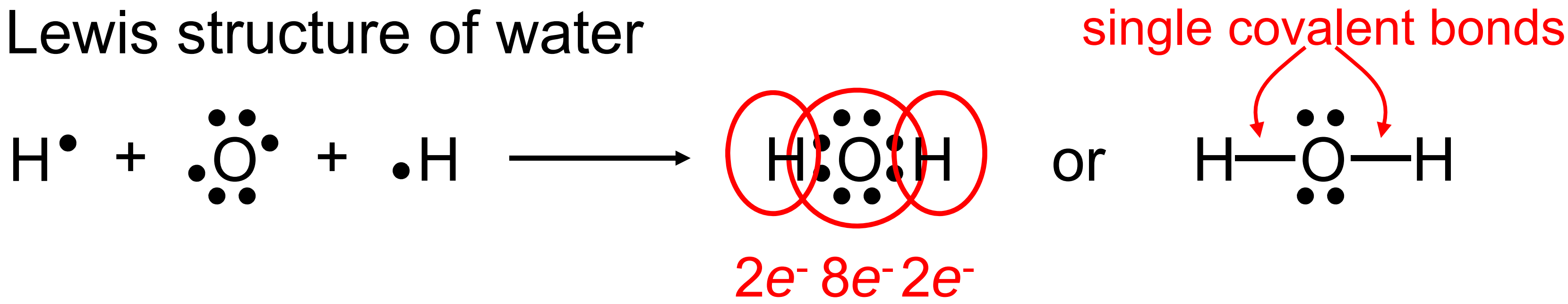
EXAMPLE

- Write the Lewis structure for nitrogen trifluoride (NF_3, a colorless, odorless, unreactive gas).

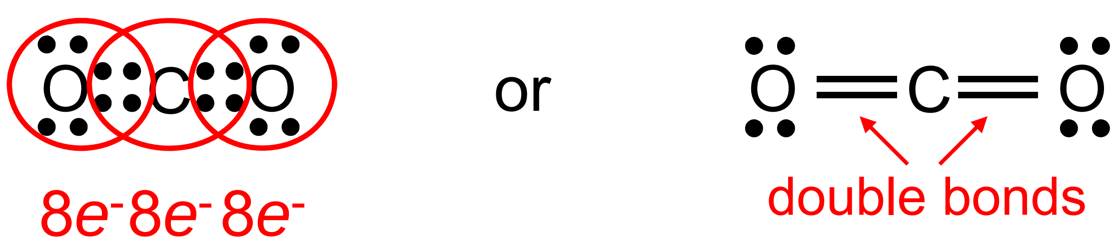


SINGLE, DOUBLE, AND TRIPLE BONDS

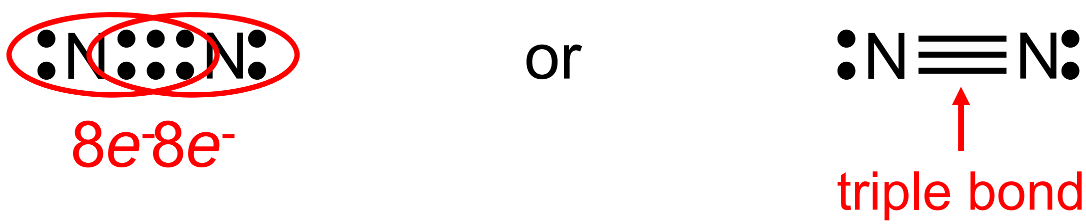
Lewis structure of water



Double bond – two atoms share two pairs of electrons

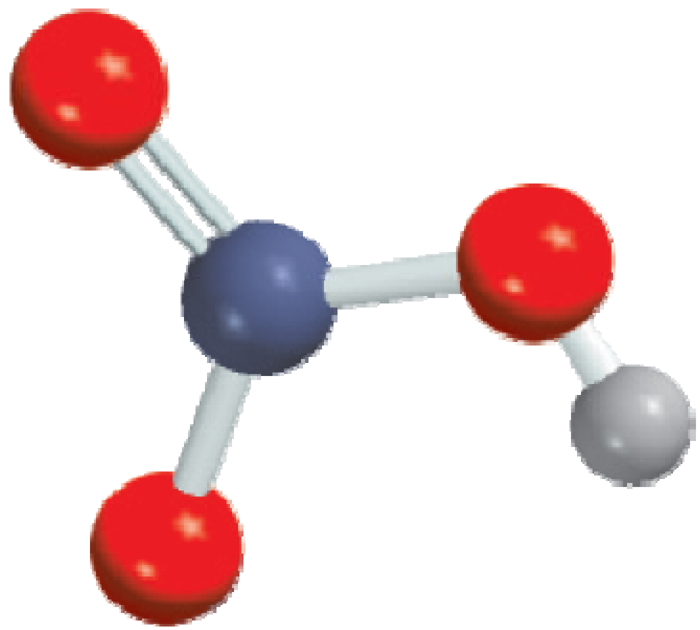


Triple bond – two atoms share three pairs of electrons



EXAMPLE

- Write the Lewis structure for nitric acid (HNO_3, a strong acid/strong electrolyte) in which the three O atoms are bonded to the central N atom and the ionizable H atom is bonded to one of the O atoms.



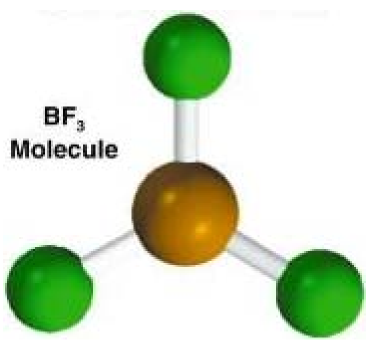
EXCEPTIONS TO THE OCTET RULE

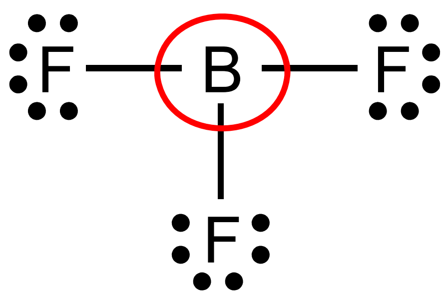
- The incomplete octet
  - While H and He get a “duet,” other elements have neither 2 nor 8 in their structures (generally unstable)

BeH_2

H—Be—H

BF_3

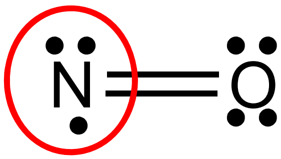




EXCEPTIONS (CONT'D)

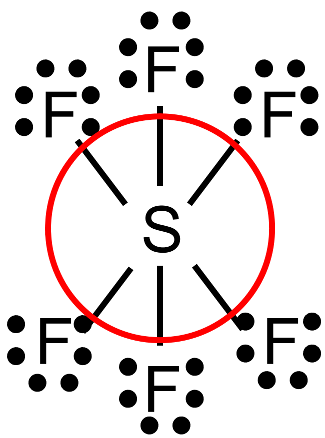
- Odd electron structures (also highly reactive)

NO



- Expanded octet
  - (central atom with principal quantum number n > 2 **ONLY**)

SF_6

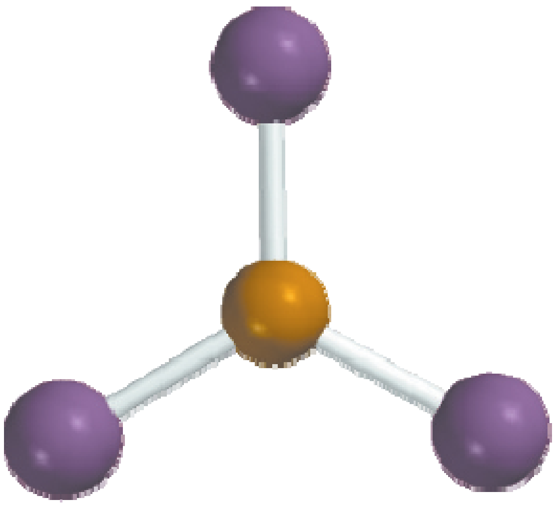


O_3 VS SO_2

The internet is wrong…

EXAMPLE

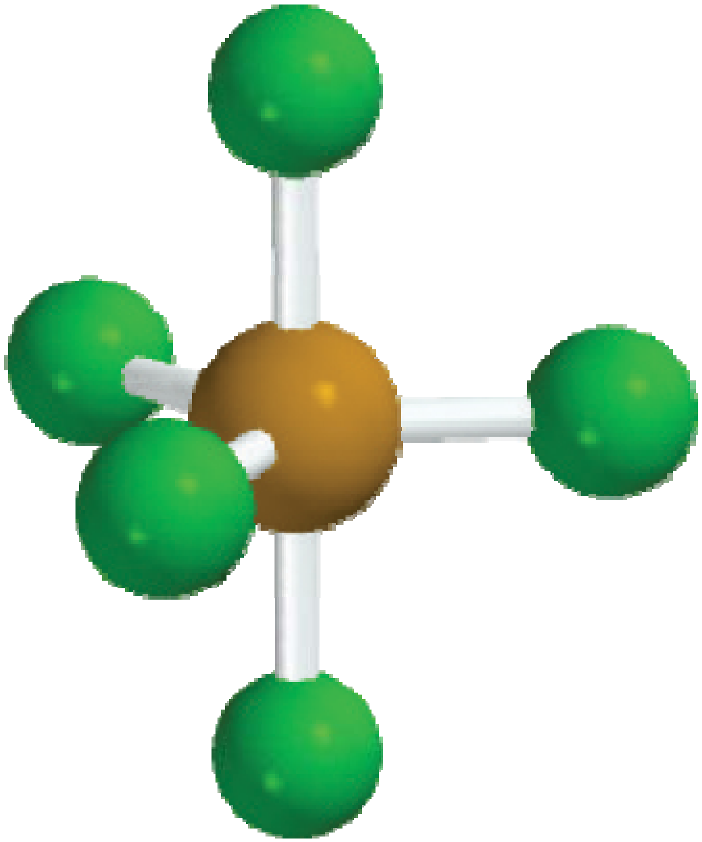
- Draw the Lewis structure for aluminum triiodide (AlI_3).



AlI_3 has a tendency to dimerize (form two units) forming Al_2I_6 (similar to many boron compounds).

EXAMPLE

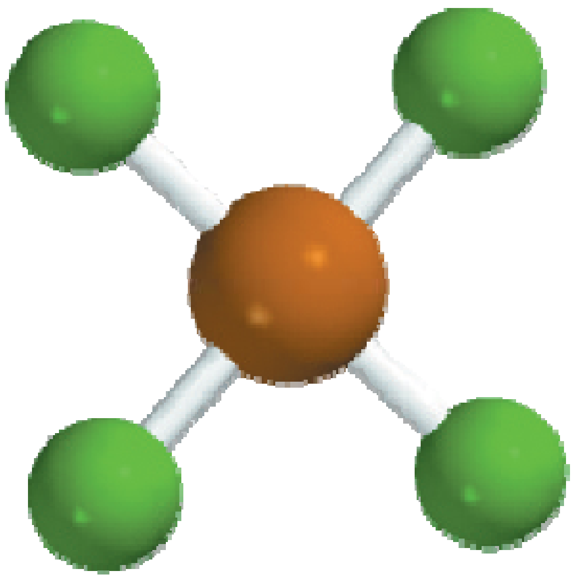
- Draw the Lewis structure for phosphorus pentafluoride (PF_5).

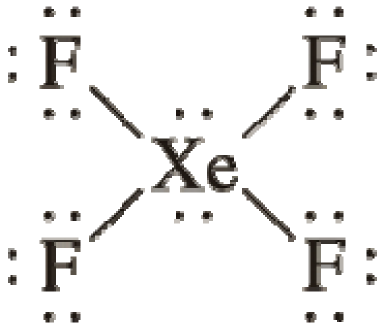


PF_5 is a reactive gaseous compound.

EXAMPLE

- Draw a Lewis structure of the noble gas compound xenon tetrafluoride (XeF_4).





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FORMAL CHARGE

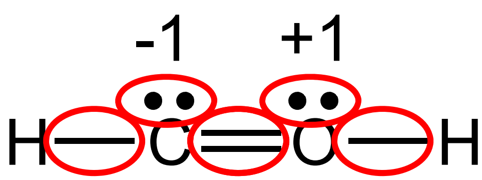
- An atom’s formal charge is the difference between the number of valence electrons in an isolated atom and the number of electrons “assigned” to that atom in a Lewis structure.
- Overly complicated method:

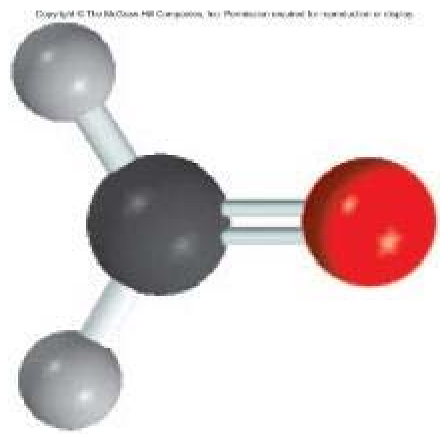
$$\text{formal charge on an atom in a Lewis structure} = \text{total number of valence electrons in the free atom} - \text{total number of nonbonding electrons} - \frac{1}{2}\left(\text{total number of bonding electrons}\right)$$

The sum of the formal charges of the atoms in a molecule or ion must equal the charge on the molecule or ion.

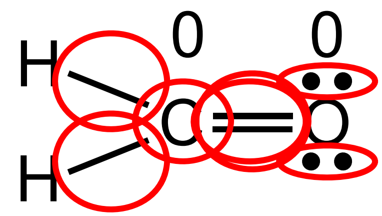
FORMAL CHARGE IN FORMALDEHYDE

Two possible skeletal structures of formaldehyde (CH_2O)





CH_2O



formal charge on C $= 4 - 2 - \frac{1}{2} \times 6 = -1$

formal charge on O $= 6 - 2 - \frac{1}{2} \times 6 = +1$

formal charge on C $= 4 - 0 - \frac{1}{2} \times 8 = 0$

formal charge on O $= 6 - 4 - \frac{1}{2} \times 4 = 0$

The best Lewis structure minimizes formal charges.

FORMAL CHARGE AND LEWIS STRUCTURES

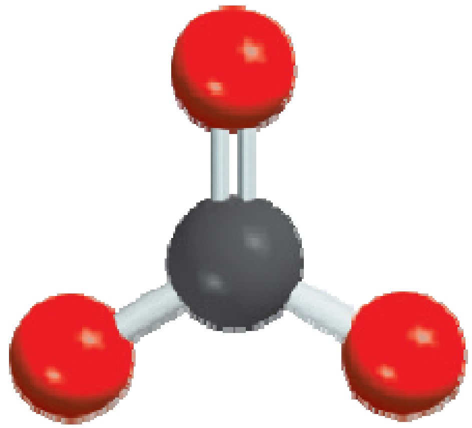
- For neutral molecules, a Lewis structure in which there are no formal charges is preferable to one in which formal charges are present.

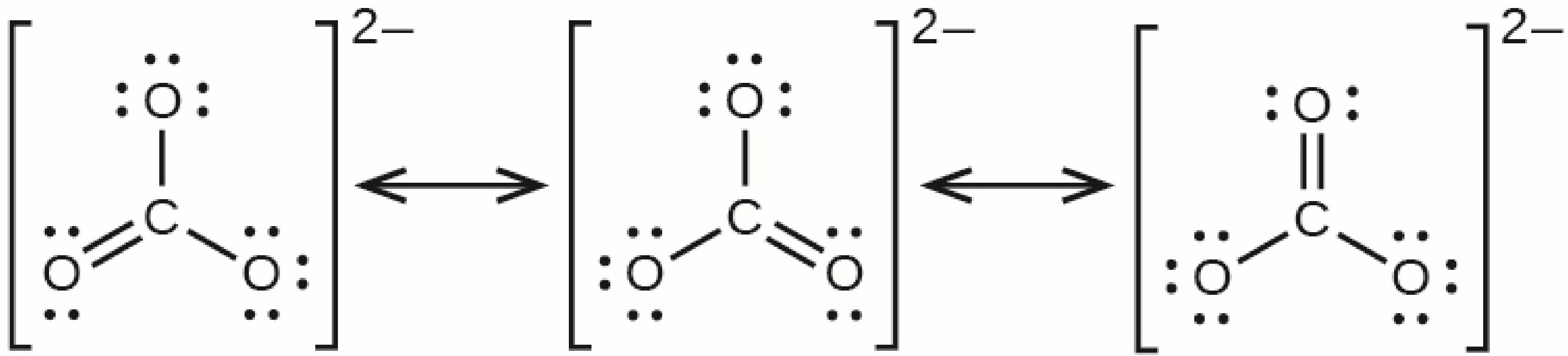
- Lewis structures with small formal charges are preferable to those with large formal charges.

- Among Lewis structures having similar distributions of formal charges, the most plausible structure is the one in which negative formal charges are placed on the more electronegative atoms.

EXAMPLE

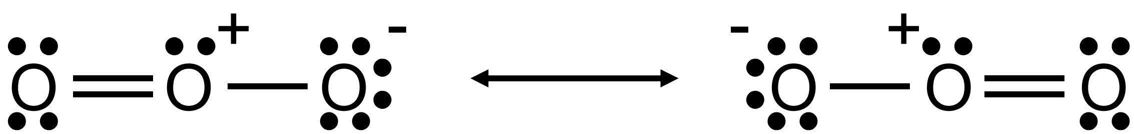
Write the Lewis structure for the carbonate ion (CO_3^{2-}).



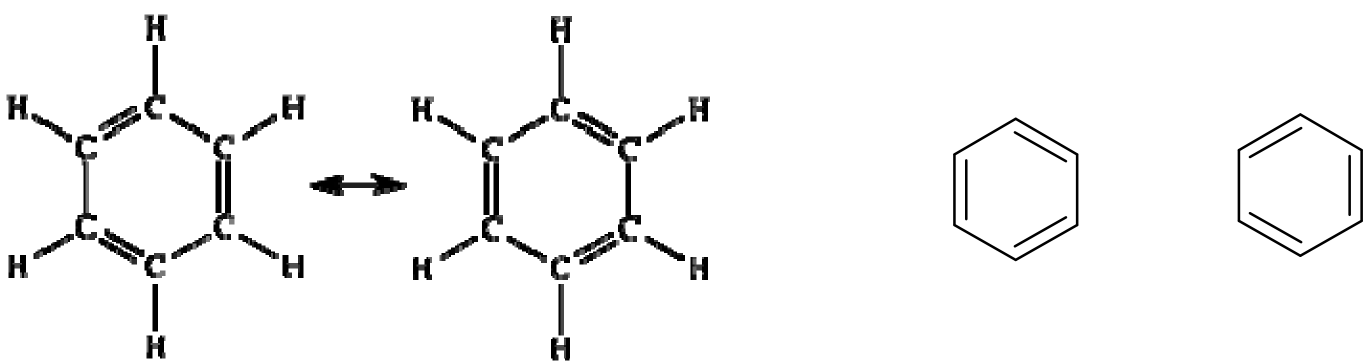


RESONANCE STRUCTURES

- A resonance structure is one of two or more Lewis structures for a single molecule that cannot be represented accurately by only one Lewis structure.
- Ozone (O_3):

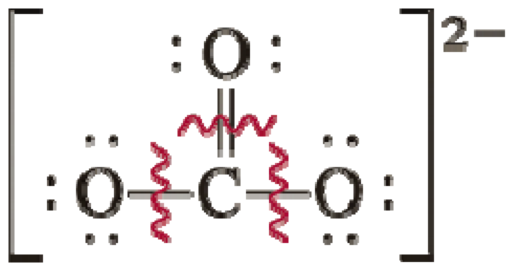


- Benzene (C_6H_6):



EXAMPLE

Write formal charges for one of the resonance forms of the carbonate ion.



Check Note that the sum of the formal charges is −2, the same as the charge on the carbonate ion.

EXAMPLE

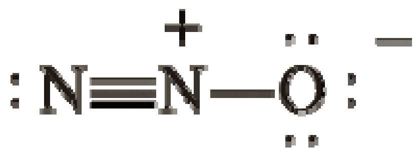
- Draw three resonance structures for the molecule nitrous oxide, N_2O (the atomic arrangement is NNO).
- Indicate formal charges.
- Rank the structures in their relative importance to the overall properties of the molecule.

SOLUTION

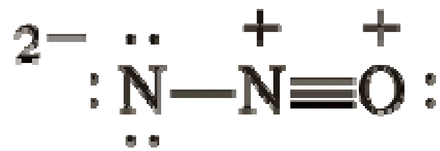
N N O

Solution The three resonance structures are

(a)



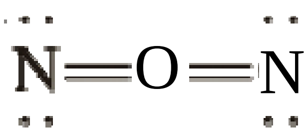
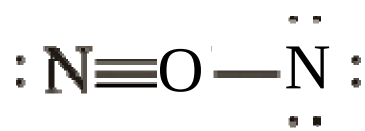
(b)



(c)

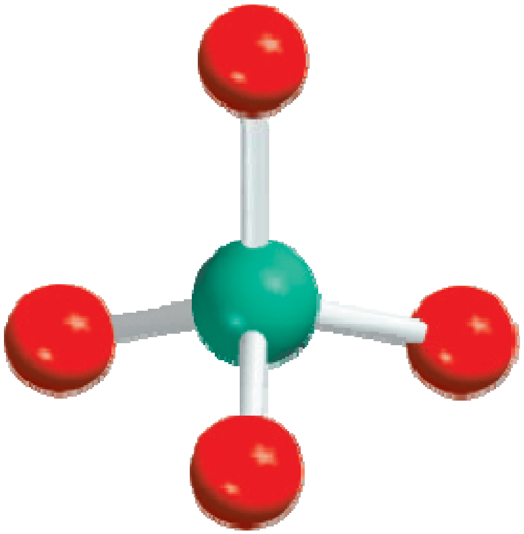
Structure (b) is the most important one because the negative charge is on the more electronegative oxygen atom.

Structure (c) is the least important one because it has a larger separation of formal charges. Also, the positive charge is on the more electronegative oxygen atom.

How about   ?

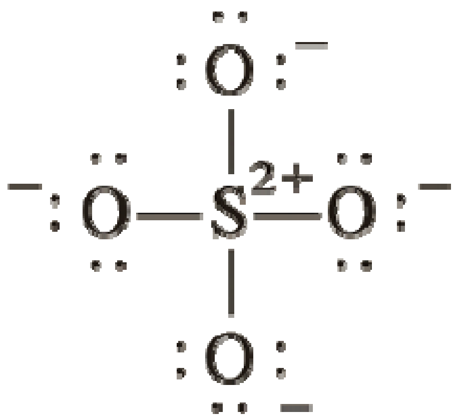
EXAMPLE

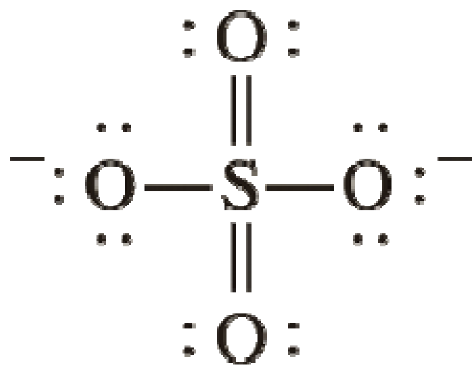
- Draw a Lewis structure for the sulfate ion (SO_4^{2-}).

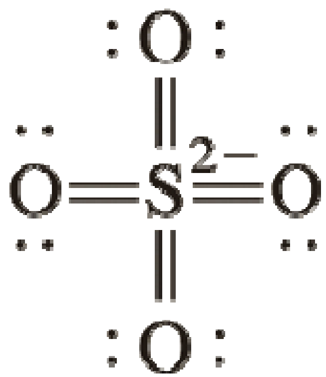


SOLUTION

The question of which of these two structures is more important, that is, the one in which the S atom obeys the octet rule but bears more formal charges or the one in which the S atom expands its octet, has been the subject of some debate among chemists. In many cases, only elaborate quantum mechanical calculations can provide a clearer answer.







At this stage of learning, you should realize that both representations are valid Lewis structures and you should be able to draw both types of structures. One helpful rule is that in trying to minimize formal charges by expanding the central atom's octet, only add enough double bonds to make the formal charge on the central atom zero.

16 electrons is…unusual.

CH. 7 OUTLINE

7.3 Lewis Symbols

7.1 Ionic Bonding

7.2 Covalent Bonding

7.3 Lewis Structures

7.4 Formal Charges and Resonance

7.5 Strengths of Ionic and Covalent Bonds

7.6 Molecular Structure and Polarity

BOND ENERGY

The enthalpy change required to break a particular bond in one mole of gaseous molecules is the bond enthalpy. (I know we skipped Chapter 6...)

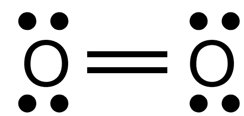
<u>Bond Enthalpy</u>

$H_{2\,(g)} \longrightarrow H_{(g)} + H_{(g)}$ $\quad \Delta H^0 = 436.4\ \text{kJ}$

$Cl_{2\,(g)} \longrightarrow Cl_{(g)} + Cl_{(g)}$ $\quad \Delta H^0 = 242.7\ \text{kJ}$

$HCl_{(g)} \longrightarrow H_{(g)} + Cl_{(g)}$ $\quad \Delta H^0 = 431.9\ \text{kJ}$

$O_{2\,(g)} \longrightarrow O_{(g)} + O_{(g)}$ $\quad \Delta H^0 = 498.7\ \text{kJ}$



$N_{2\,(g)} \longrightarrow N_{(g)} + N_{(g)}$ $\quad \Delta H^0 = 941.4\ \text{kJ}$

Bond Enthalpies

Single bond < Double bond < Triple bond

BOND ENERGIES

- Tabulated bond energy values are average bond enthalpies in polyatomic molecules

$$H_2O_{(g)} \longrightarrow H_{(g)} + OH_{(g)} \quad \Delta H^0 = 502 \text{ kJ}$$

$$OH_{(g)} \longrightarrow H_{(g)} + O_{(g)} \quad \Delta H^0 = 427 \text{ kJ}$$

$$\text{Average OH bond enthalpy} = \frac{502 + 427}{2}$$

Table 9.4 Some Bond Enthalpies of Diatomic Molecules* and Average Bond Enthalpies for Bonds in Polyatomic Molecules

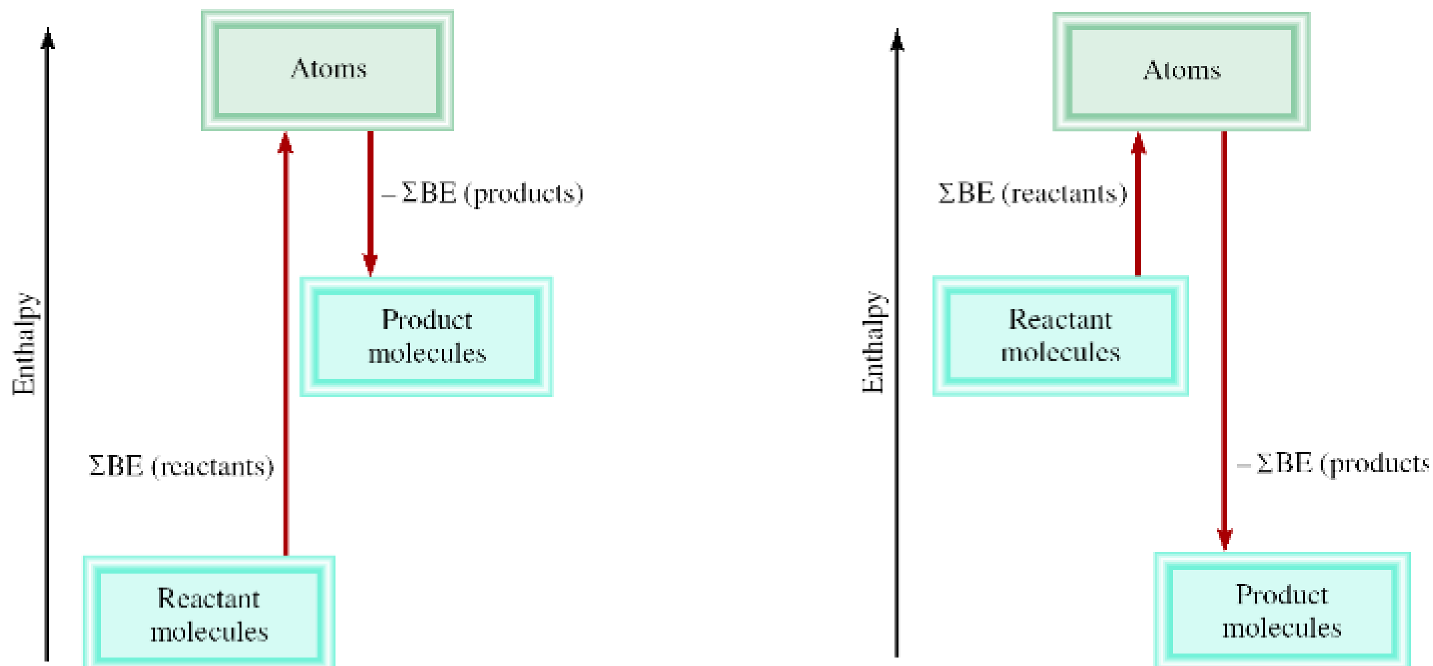
Bond	Bond Enthalpy (kJ/mol)	Bond	Bond Enthalpy (kJ/mol)
H—H	436.4	C—I	240
H—N	393	C—P	263
H—O	460	C—S	255
H—S	368	C═S	477
H—P	326	N—N	193
H—F	568.2	N═N	418
H—Cl	431.9	N≡N	941.4
H—Br	366.1	N—O	176
H—I	298.3	N═O	607
C—H	414	O—O	142
C—C	347	O═O	498.7
C═C	620	O—P	502
C≡C	812	O═S	469
C—N	276	P—P	197
C═N	615	P═P	489
C≡N	891	S—S	268
C—O	351	S═S	352
C═O†	745	F—F	156.9
C≡O	1076.5	Cl—Cl	242.7
C—F	450	Br—Br	192.5
C—Cl	338	I—I	151.0
C—Br	276		

*Bond enthalpies for diatomic molecules (in color) have more significant figures than bond enthalpies for bonds in polyatomic molecules because the bond enthalpies of diatomic molecules are directly measurable quantities and not averaged over many compounds.
†The C═O bond enthalpy in CO_2 is 799 kJ/mol.

HEAT OF REACTION

- Imagine a reaction proceeding by breaking all bonds (takes E) in the reactants and then using the gaseous atoms to form all the bonds (releases E) in the products.

$$\Delta H^0 = \text{total energy input} - \text{total energy released}$$
$$= \Sigma BE(\text{reactants}) - \Sigma BE(\text{products})$$

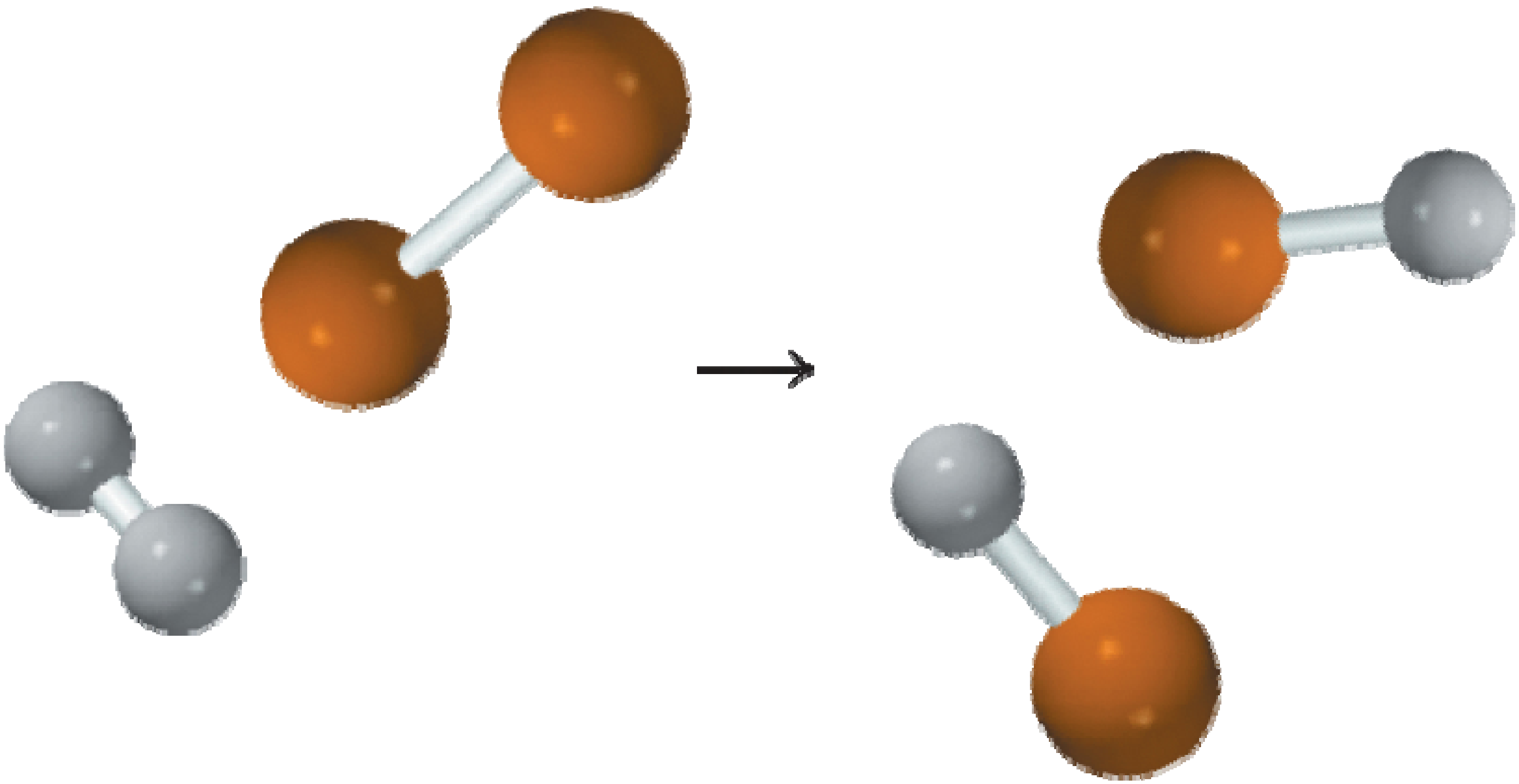


endothermic exothermic

EXAMPLE

Calculate the enthalpy of reaction for the process

$$H_2(g) + Cl_2(g) \longrightarrow 2HCl(g)$$



SOLUTION

Start by counting the number of bonds broken and the number of bonds formed and the corresponding energy changes:

Type of bonds broken	*Number of bonds broken*	*Bond enthalpy (kJ/mol)*	*Energy change (kJ/mol)*
H—H (H_2)	1	436.4	436.4
Cl—Cl (Cl_2)	1	242.7	242.7

Type of bonds formed	*Number of bonds formed*	*Bond enthalpy (kJ/mol)*	*Energy change (kJ/mol)*
H—Cl (HCl)	2	431.9	863.8

Next, obtain the total energy input and total energy released:

$$\text{total energy input} = 436.4 \text{ kJ/mol} + 242.7 \text{ kJ/mol} = 679.1 \text{ kJ/mol}$$
$$\text{total energy released} = 863.8 \text{ kJ/mol}$$

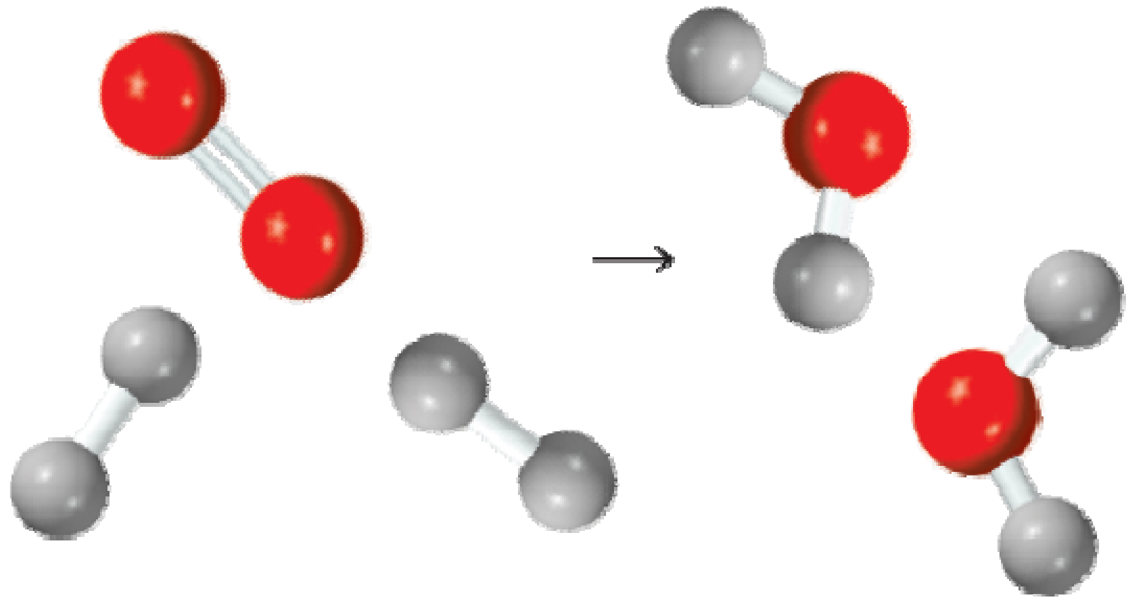
And finally, find the heat of reaction:

$$\Delta H^\circ = 679.1 \text{ kJ/mol} - 863.8 \text{ kJ/mol} = -184.7 \text{ kJ/mol}$$

EXAMPLE

Estimate the enthalpy change for the combustion of hydrogen gas:

$$2H_2(g) + O_2(g) \longrightarrow 2H_2O(g)$$



SOLUTION

Type of bonds broken	*Number of bonds broken*	*Bond enthalpy (kJ/mol)*	*Energy change (kJ/mol)*
H—H (H_2)	2	436.4	872.8
O=O (O_2)	1	498.7	498.7

Type of bonds formed	*Number of bonds formed*	*Bond enthalpy (kJ/mol)*	*Energy change (kJ/mol)*
O—H (H_2O)	4	460	1840

Obtain the total energy input and total energy released:

$$\text{total energy input} = 872.8 \text{ kJ/mol} + 498.7 \text{ kJ/mol} = 1371.5 \text{ kJ/mol}$$

$$\text{total energy released} = 1840 \text{ kJ/mol}$$

Thus,

$$\Delta H° = 1371.5 \text{ kJ/mol} - 1840 \text{ kJ/mol} = -469 \text{ kJ/mol}$$

ELECTROSTATIC (LATTICE) ENERGY

- Lattice energy (U) is the energy required to completely separate one mole of a solid ionic compound into gaseous ions.

$$E = k\frac{Q_+Q_-}{r}$$

E is the potential energy

Q_+ is the charge on the cation

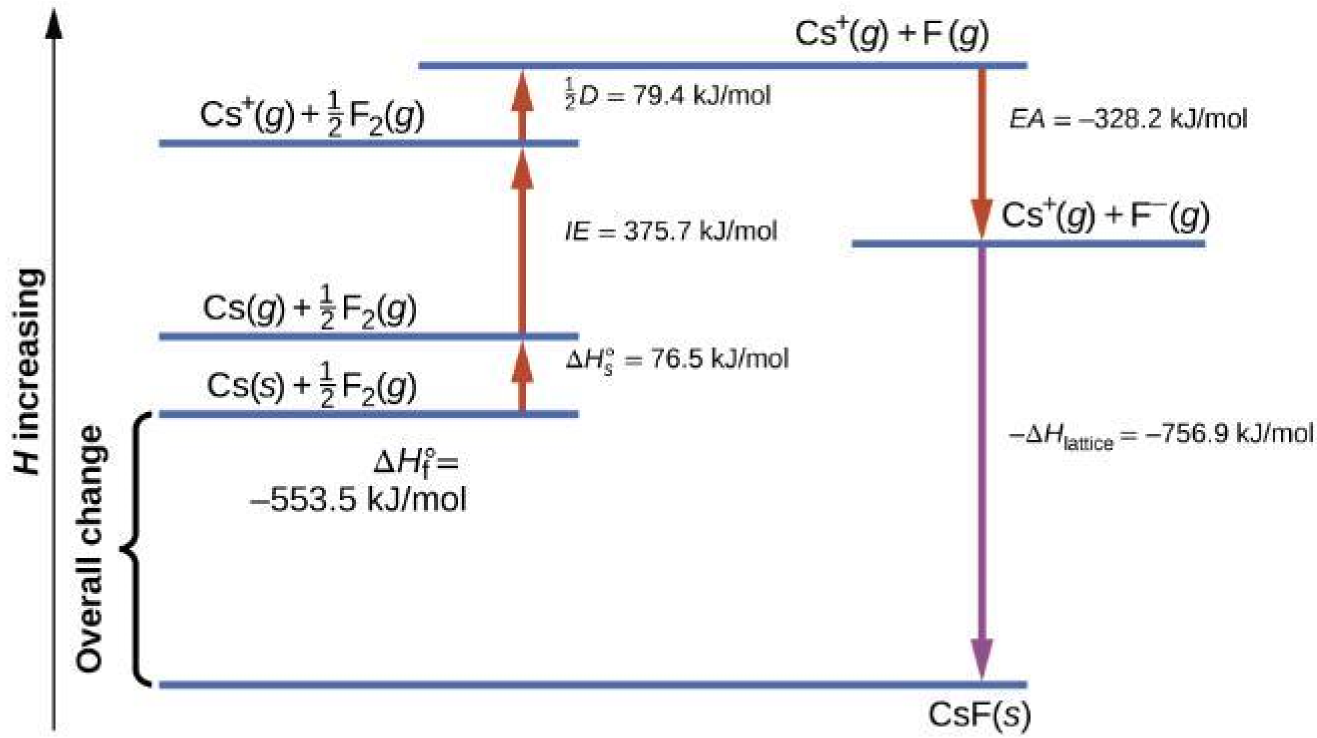
Q_- is the charge on the anion

r is the distance between the ions

Lattice energy increases as *Q increases* and/or as *r decreases*.

Compound	Lattice Energy (kJ/mol)	
MgF_2	2957	*Q:* +2,-1
MgO	3938	*Q:* +2,-2
LiF	1036	*r* F^- < *r* Cl^-
LiCl	853	

FIGURE 7.13



The Born-Haber cycle shows the relative energies of each step involved in the formation of an ionic solid from the necessary elements in their reference states.

$$\Delta H^o_{overall} = \Delta H^o_1 + \Delta H^o_2 + \Delta H^o_3 + \Delta H^o_4 + \Delta H^o_5$$

LATTICE ENERGIES

Compound	Lattice Energy (kJ/mol)	Melting Point (°C)
LiF	1017	845
LiCl	828	610
LiBr	787	550
LiI	732	450
NaCl	788	801
NaBr	736	750
NaI	686	662
KCl	699	772
KBr	689	735
KI	632	680
$MgCl_2$	2527	714
Na_2O	2570	Sub*
MgO	3890	2800
Al_2O_3	14,910	2072

*Na_2O sublimes at 1275°C.

CH. 7 OUTLINE

7.3 Lewis Symbols

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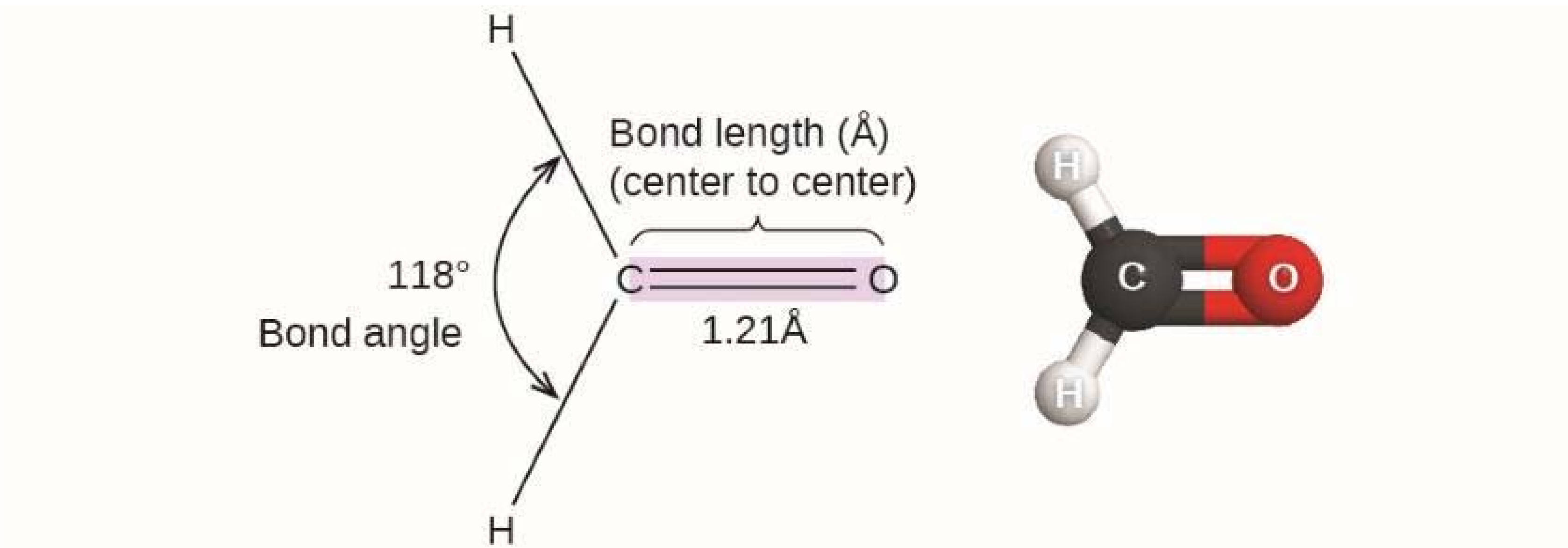
MOVING FROM 2D LEWIS TO 3D SHAPE

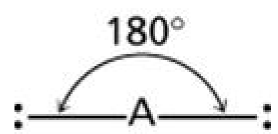


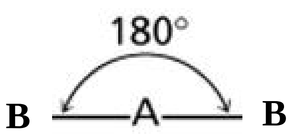
Bond distances (lengths) and angles are shown for the formaldehyde molecule, H_2CO.

VSEPR THEORY

Valence Shell Electron Pair Repulsion theory allows us to predict the geometry of a molecule from the electrostatic repulsions between the electron (bonding and nonbonding) pairs

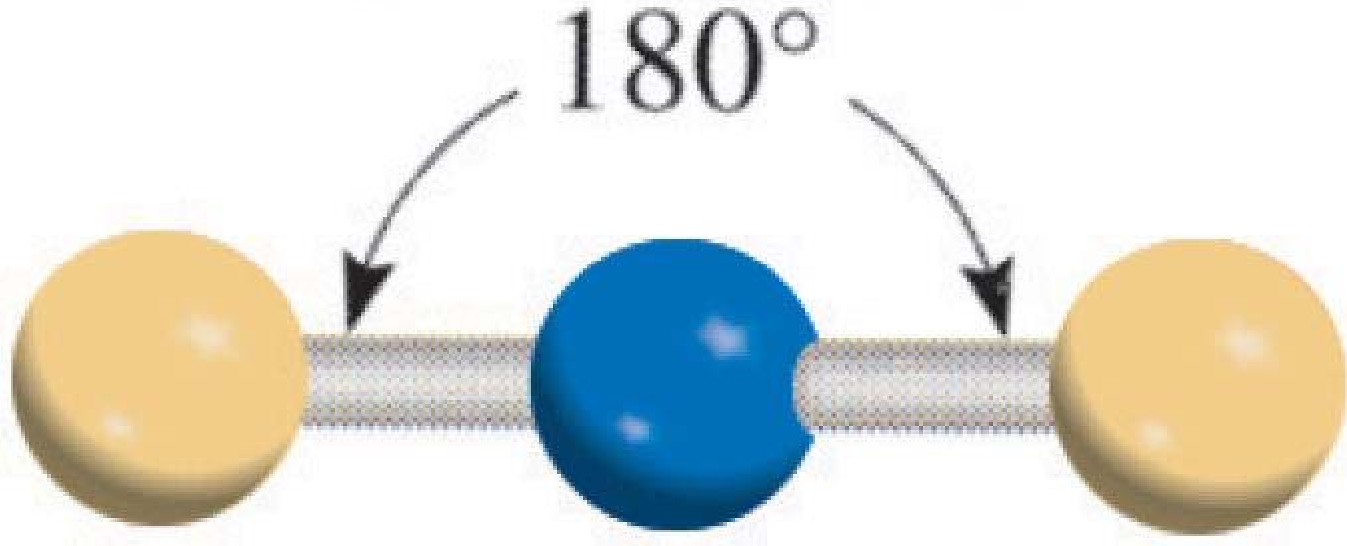
~~Class~~	# of atoms bonded to central atom	# lone pairs on central atom	Geometry of electron groups	Shape of the molecule
$\cancel{AB_2}$	2	0	linear	linear



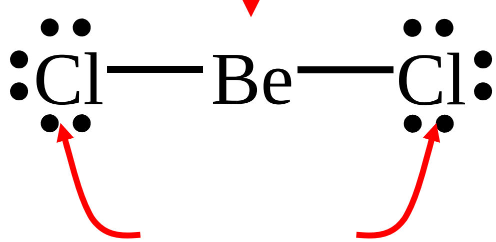


EXAMPLE

Beryllium chloride



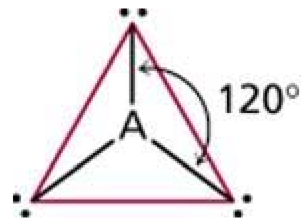
0 lone pairs on central atom

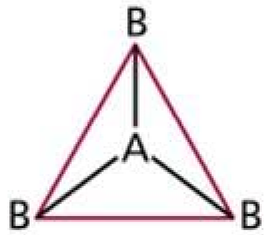


2 atoms bonded to central atom

3 BONDED ATOMS

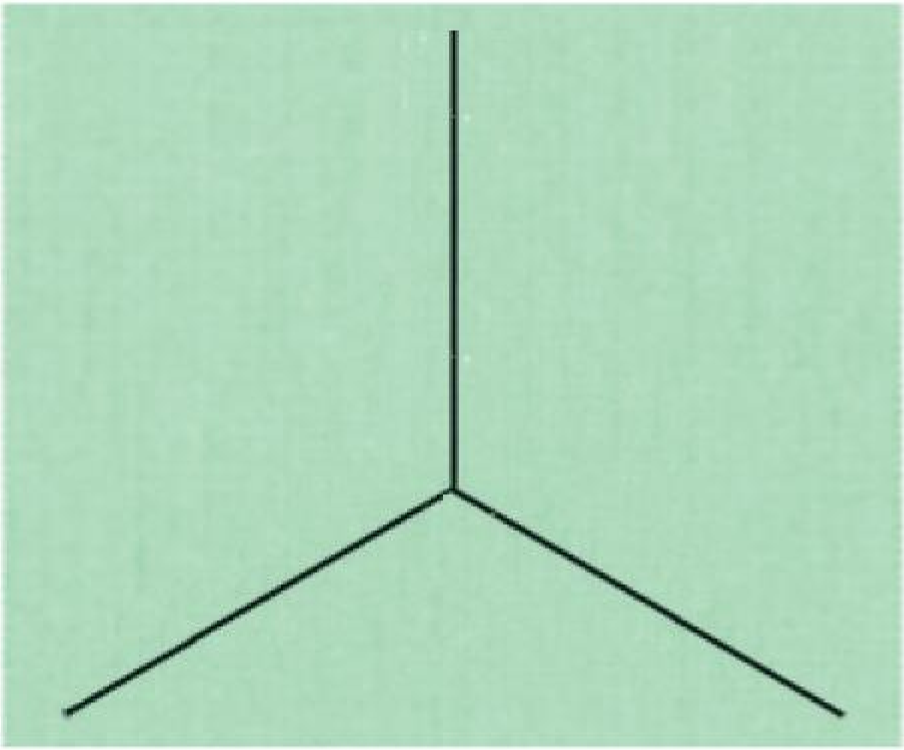
Class	# of atoms bonded to central atom	# lone pairs on central atom	Geometry of electron groups	Shape of the molecule
AB_2	2	0	linear	linear
AB_3	3	0	trigonal planar	trigonal planar



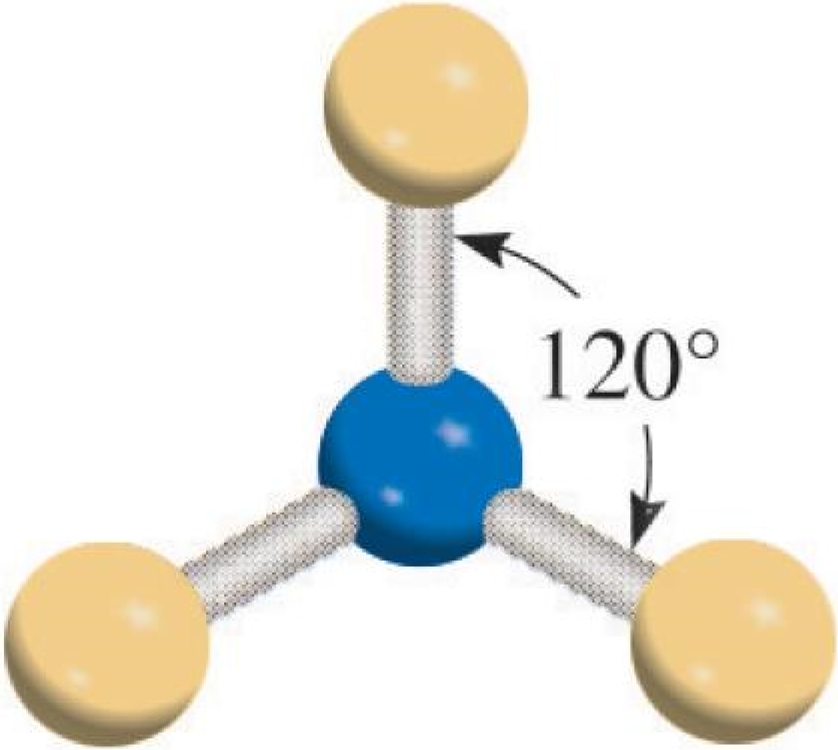


EXAMPLE

Boron trifluoride

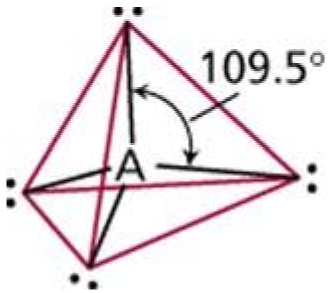


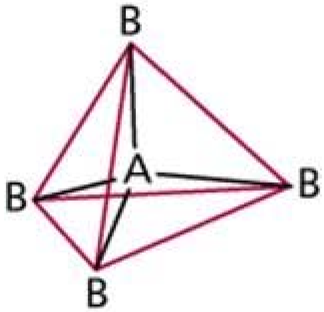
Planar



4 BONDED ATOMS

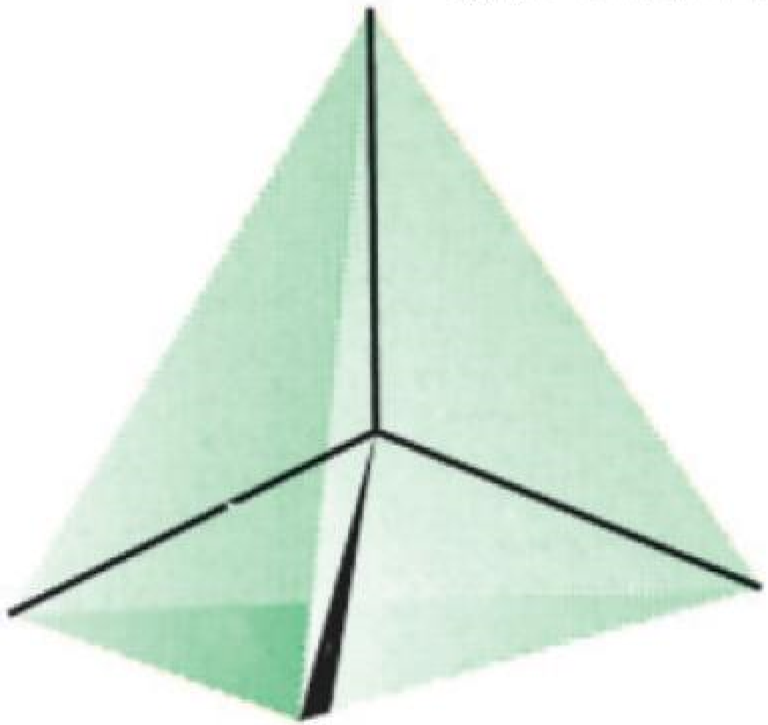
Class	# of atoms bonded to central atom	# lone pairs on central atom	Geometry of electron groups	Shape of the molecule
~~AB_2~~	2	0	linear	linear
~~AB_3~~	3	0	trigonal planar	trigonal planar
AB_4	4	0	tetrahedral	tetrahedral



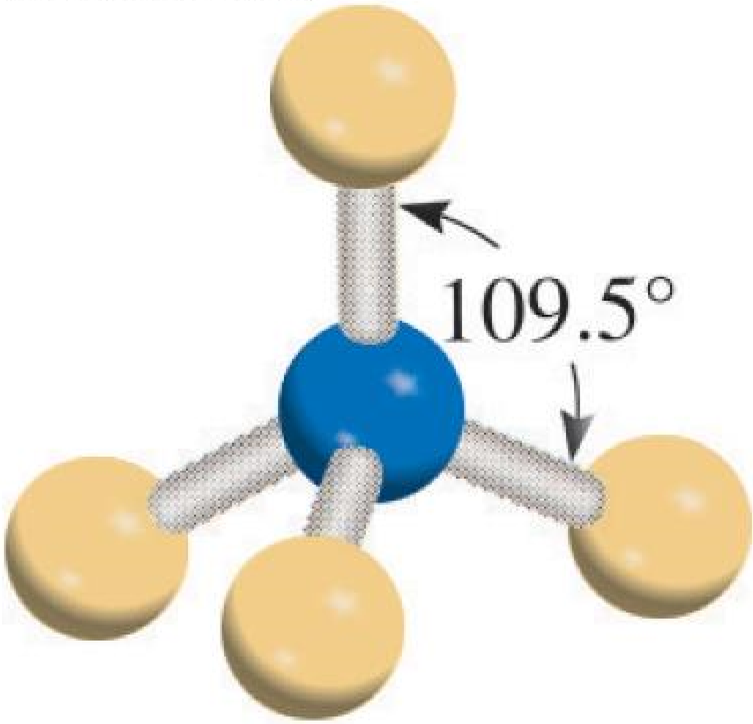


EXAMPLE

Methane

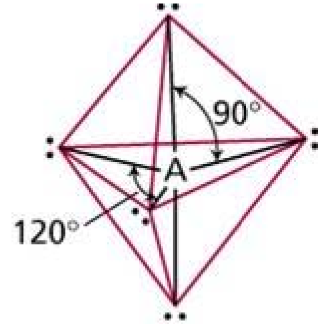


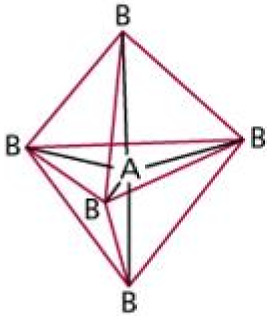
Tetrahedral



5 BONDED ATOMS

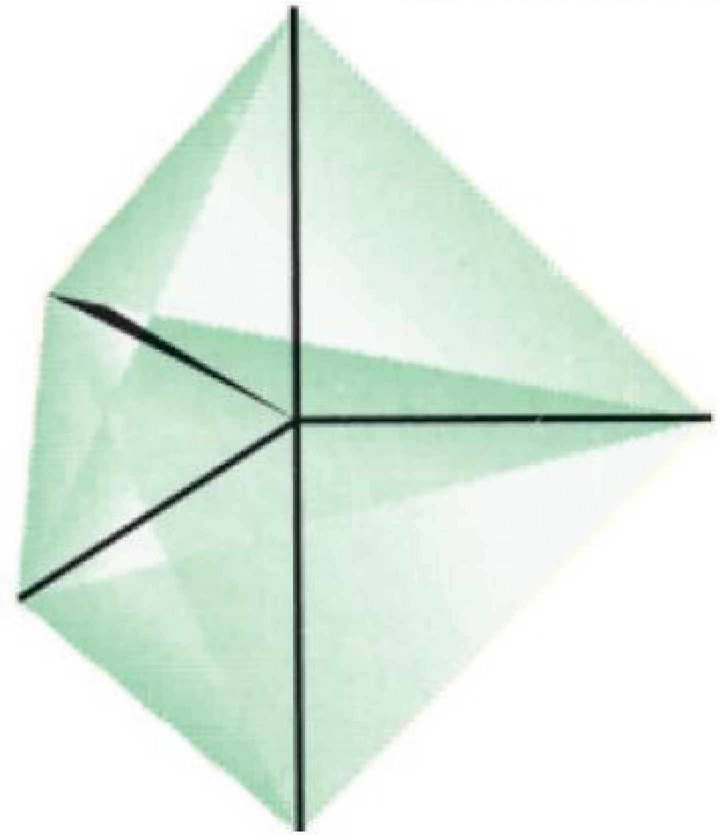
Class	# of atoms bonded to central atom	# lone pairs on central atom	Geometry of electron groups	Shape of the molecule
~~AB_2~~	2	0	linear	linear
~~AB_3~~	3	0	trigonal planar	trigonal planar
~~AB_4~~	4	0	tetrahedral	tetrahedral
~~AB_5~~	5	0	trigonal bipyramidal	trigonal bipyramidal



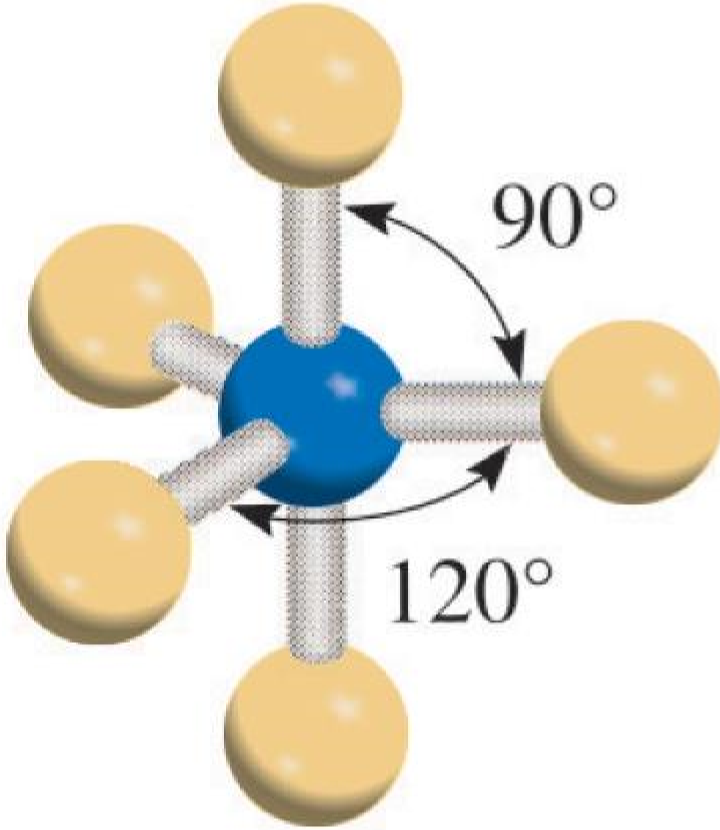


EXAMPLE

Phosphorus pentachloride

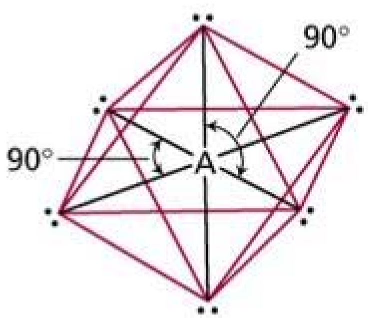


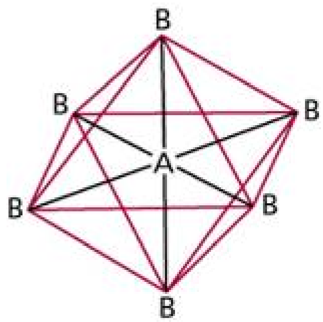
Trigonal bipyramidal



6 BONDED ATOMS

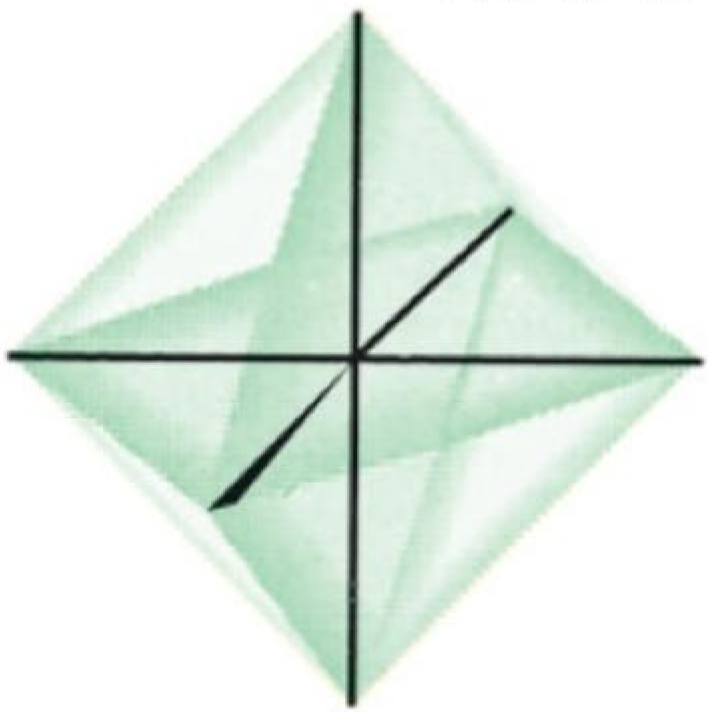
Class	# of atoms bonded to central atom	# lone pairs on central atom	Geometry of electron groups	Shape of the molecule
AB_2	2	0	linear	linear
AB_3	3	0	trigonal planar	trigonal planar
AB_4	4	0	tetrahedral	tetrahedral
AB_5	5	0	trigonal bipyramidal	trigonal bipyramidal
AB_6	6	0	octahedral	octahedral



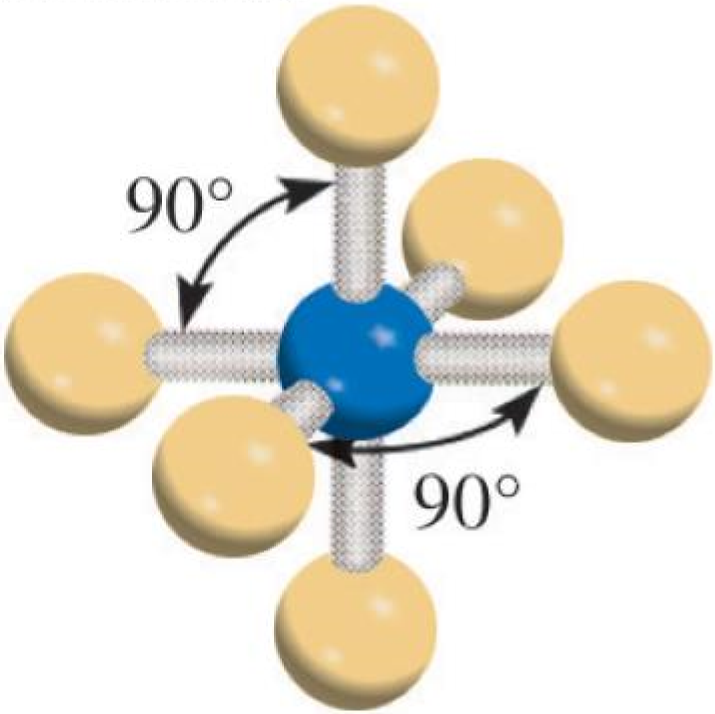


EXAMPLE

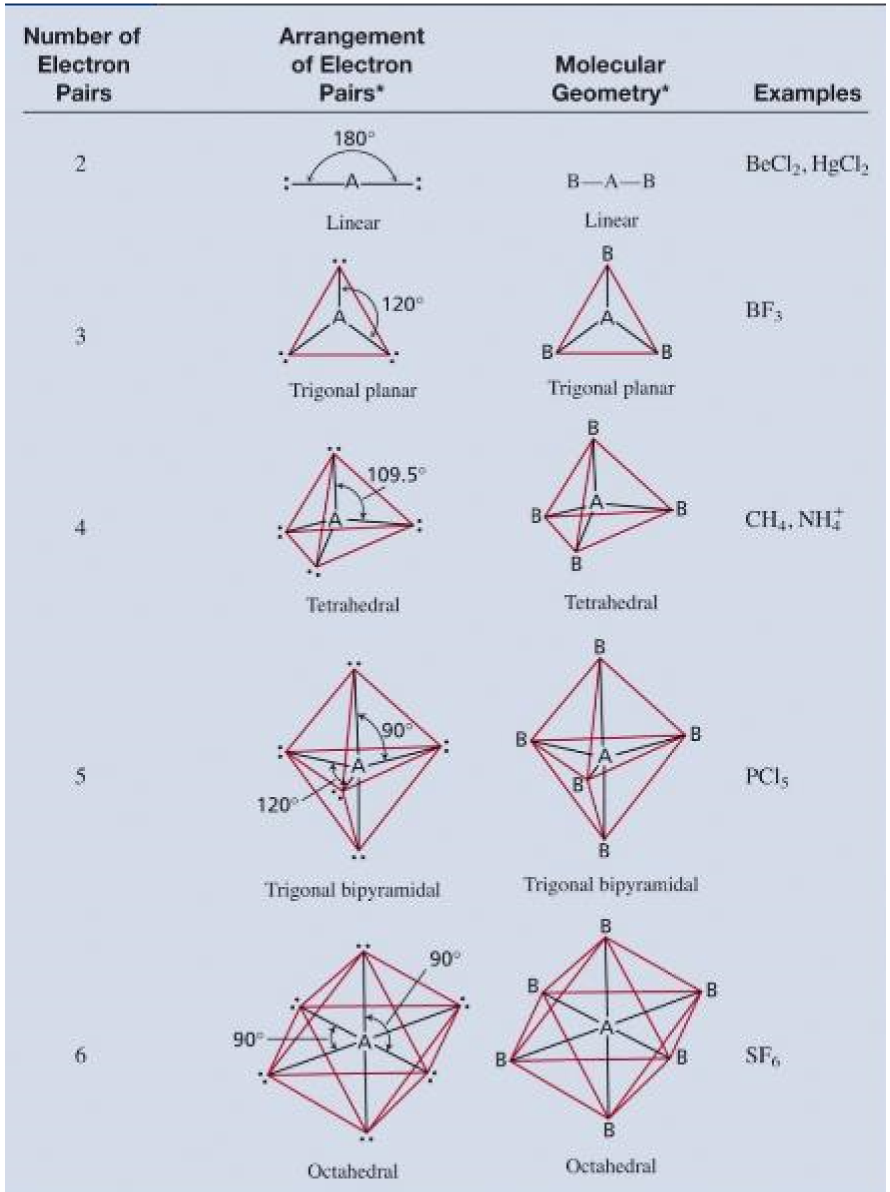
Sulfur hexafluoride



Octahedral



SUMMARY – VSEPR - NO LONE PAIRS

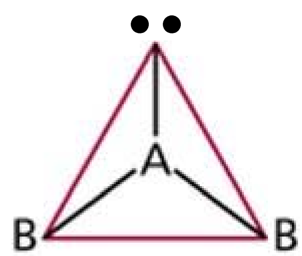


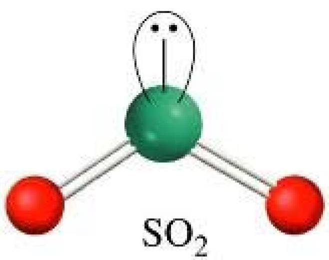
Number of Electron Pairs	Arrangement of Electron Pairs*	Molecular Geometry*	Examples
2	180° Linear	B—A—B Linear	$BeCl_2$, $HgCl_2$
3	120° Trigonal planar	Trigonal planar	BF_3
4	109.5° Tetrahedral	Tetrahedral	CH_4, NH_4^+
5	90° 120° Trigonal bipyramidal	Trigonal bipyramidal	PCl_5
6	90° 90° Octahedral	Octahedral	SF_6

*The colored lines are used only to show the overall shapes; they do not represent bonds.

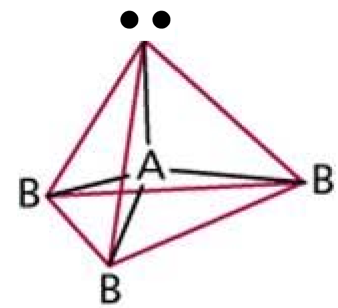
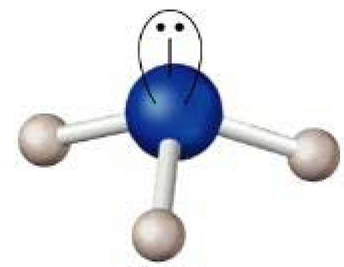
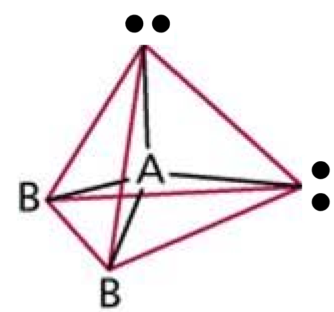
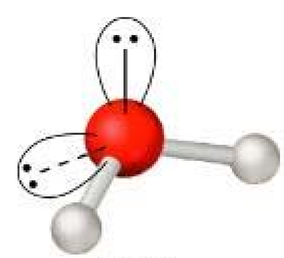
2 BONDED PAIRS; 1 LONE PAIR

Class	# of atoms bonded to central atom	# lone pairs on central atom	Geometry of electron groups	Shape of the molecule
AB_3	3	0	trigonal planar	trigonal planar
AB_2E	2	1	trigonal planar	bent

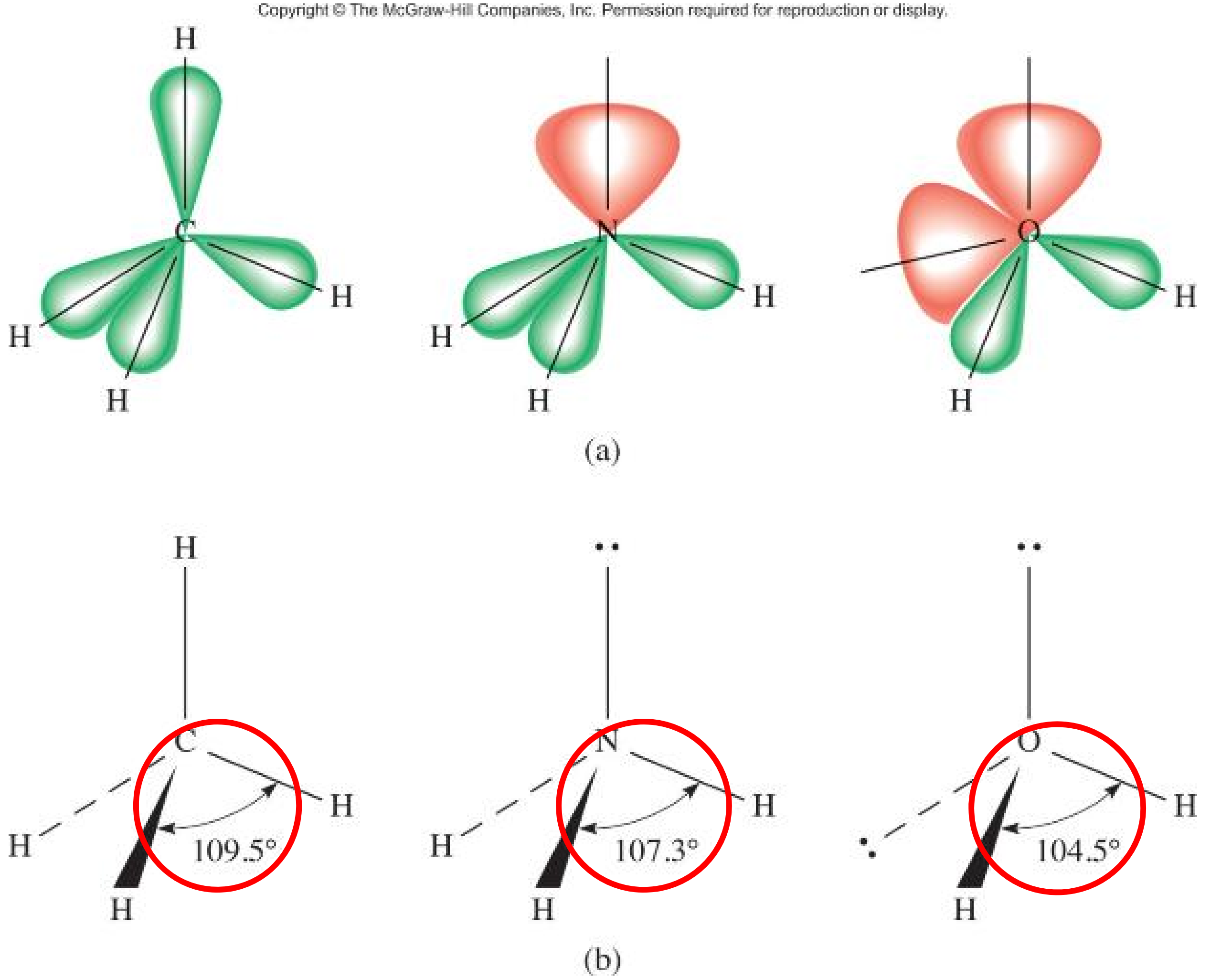




4 ELECTRON GROUPS

Class	# of atoms bonded to central atom	# lone pairs on central atom	Geometry of electron groups	Shape of the molecule
AB_4	4	0	tetrahedral	tetrahedral
AB_3E	3	1	tetrahedral 	trigonal pyramidal  NH_3
AB_2E_2	2	2	tetrahedral 	bent  H_2O

MODIFIED BOND ANGLES



bonded-pair vs. bonded-pair repulsion < lone-pair vs. bonded-pair repulsion < lone-pair vs. lone-pair repulsion

JOHN ELLIS WATER DISCOVERY

VIDEO PROOF

Norman Rockwell

and Other American Icons

These are people that influenced my life in New Rochelle, NY where Norman Rockwell lived for 25 years and where my family lived for 3 generations.

We all knew and loved the man in spite of a book trashing him in another attempt to destroy everything that is great about America! I am writing a book with a rebuttal that includes the untold stories about many others that shaped our country.

Did you ever wonder what happened to over 100 signed letters from FDR, that Harvard wanted for their archives?

Most of these people I met in my parents living room: Dr. Norman Vincent Peale, James Cash Penney, Lowell Thomas, Charles E. Wilson (Chairman of GE, FDR appointed him head of the War Production Board WW2), Carrie Chapman Catt (Woman Suffragist), Dr. James E. West (Chief Scout Executive, Boy Scouts of America), William Frank Snyder (FDR's lawyer and close friend, who also had polio, wrote his will and handled his financial affairs including Mrs. Delano, complaining to my mother: "The Roosevelt's are using my pool!"), "Buffalo Bob" Smith (It's Howdy Doody Time!), C.L. Lowes: (My grandfather started BOND BREAD. Buying trainloads of flour for 50 plants, he waited for the price of flour to go UP so farmers could make a fair profit...he was unique! General Baking Co became General Host..."Twinkies") Richard Ellis (my brother, commercial Real Estate) and many others!

After my father died, Dr. Peale said the eulogy and inspired me to increase water properties back to what it was before "The Flood" (living to Biblical ages). After "The Flood" they didn't live as long!

Since I am the first person in history to do it, should be ample proof that it had to come from divine inspiration! With an Engineering Degree that includes Steam Plant Design, I increased the Hydrogen Bond Angle (HBA) in ordinary water from 104 to 114 degrees, confirmed by scientists at Los Alamos Nuclear Lab and Lawrence Livermore to The Washington Times.

The Washington Post (on our website): "10,000 people per day" traveling to obtain water from my countertop machines, even adding water to a well with miraculous results! Dr. G. Abraham MD UCLA: "Nothing is even close for measurable Blood Flow with a 114 HBA!" At 84, MEASURE 3000% more ENERGY in your drinking water (Video)!! 13 Patents 332 FDA Tests **johnellis.com/measure**

FREE Bottled Water SAMPLE! 570.296.0214

Gilbert de Daunant (Prince Rainier's cousin):"I just walked 40 blocks and I am 94! Send another E5 to Monaco!"

THE FLOOD REVISITED

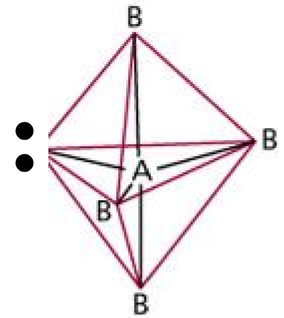
ORDER A MACHINE 845.754.8696 LISTEN TO A RECORDING 800.433.9553

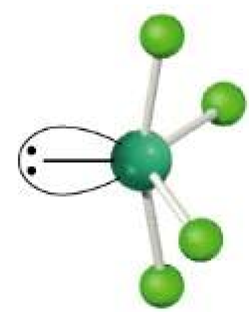
watercuresanything.com/measure

Circle #18; see card pg 81

5 ELECTRON GROUPS

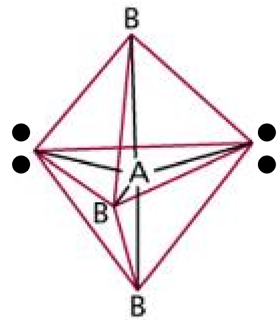
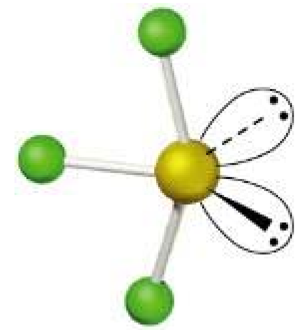
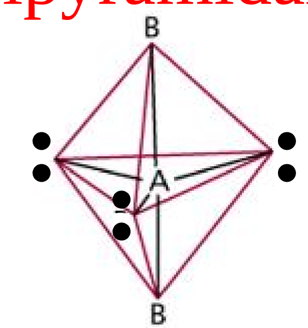
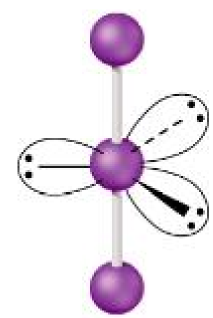
Class	# of atoms bonded to central atom	# lone pairs on central atom	**Geometry of electron groups**	**Shape of the molecule**
AB_5	5	0	trigonal bipyramidal	trigonal bipyramidal
AB_4E	4	1	trigonal bipyramid	(sawhorse) seesaw



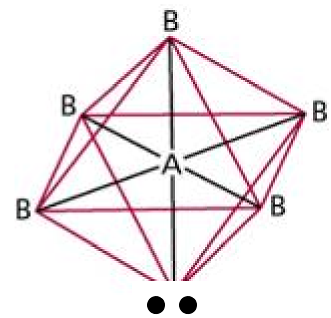
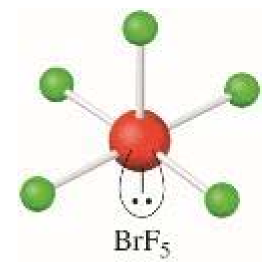
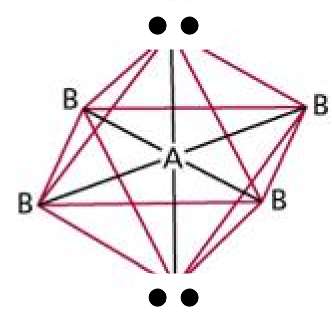
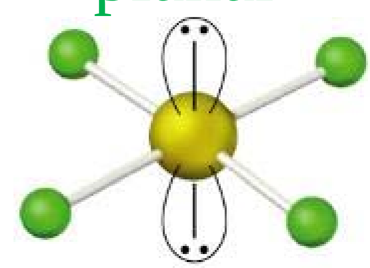


SF_4

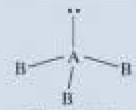
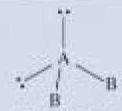
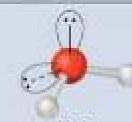
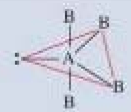
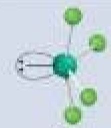
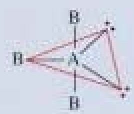
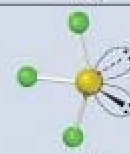
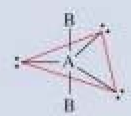
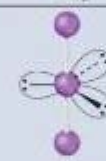
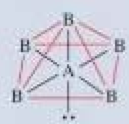
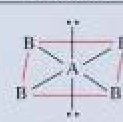
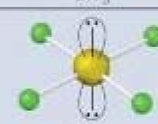
5 ELECTRON GROUPS (CONT'D)

Class	# of atoms bonded to central atom	# lone pairs on central atom	Geometry of electron groups	Shape of the molecule
AB_3E_2	3	2	trigonal bipyramidal 	T-shaped  ClF_3
AB_2E_3	2	3	trigonal bipyramidal 	linear  I_3^-

6 ELECTRON GROUPS

Class	# of atoms bonded to central atom	# lone pairs on central atom	Geometry of electron groups	Shape of the molecule
AB_6	6	0	octahedral	octahedral
AB_5E	5	1	octahedral 	square pyramidal 
AB_4E_2	4	2	octahedral 	square planar  XeF_4

VSEPR – SUMMARY WITH LP (7.19)

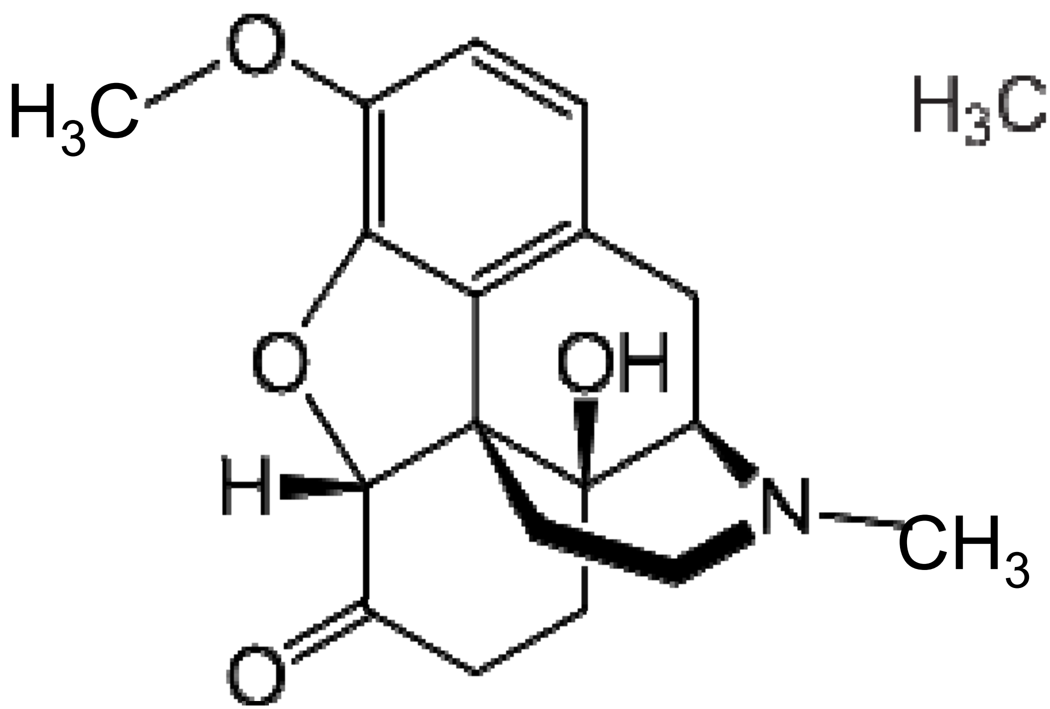
Total Number of Electron Pairs	Number of Bonding Pairs	Number of Lone Pairs	Arrangement of Electron Pairs*	Geometry of Molecule or Ion	Examples
3	2	1	 Trigonal planar	Bent	 SO_2
4	3	1	 Tetrahedral	Trigonal pyramidal	 NH_3
4	2	2	 Tetrahedral	Bent	 H_2O
5	4	1	 Trigonal bipyramidal	Distorted tetrahedron (or seesaw)	 SF_4
5	3	2	 Trigonal bipyramidal	T-shaped	 ClF_3
5	2	3	 Trigonal bipyramidal	Linear	 I_3^-
6	5	1	 Octahedral	Square pyramidal	 BrF_5
6	4	2	 Octahedral	Square planar	 XeF_4

PREDICTING MOLECULAR SHAPE

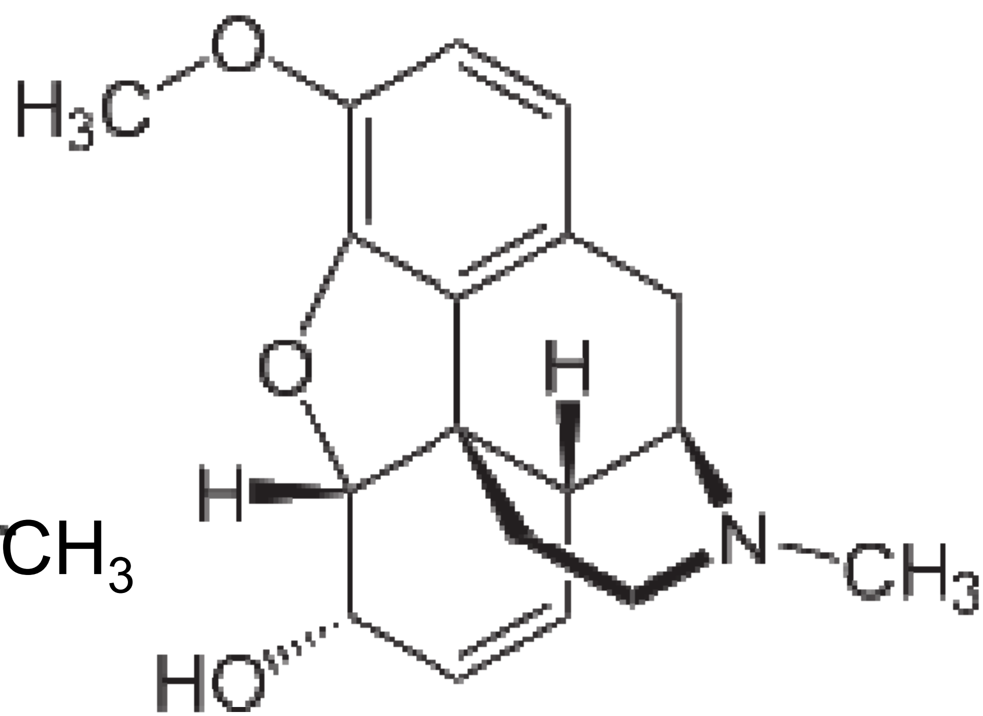
1. Draw the Lewis structure for molecule.
2. Count the number of lone pairs on the central atom and the number of atoms bonded to the central atom.
3. Use VSEPR to predict the geometry around the central atom (total number of “things”) and the shape of the molecule (total number of atoms).
   - For multi-center molecules, you’ll be describing the geometry and shape around a specific atom.

STRUCTURE DETERMINES FUNCTION

Oxycodone

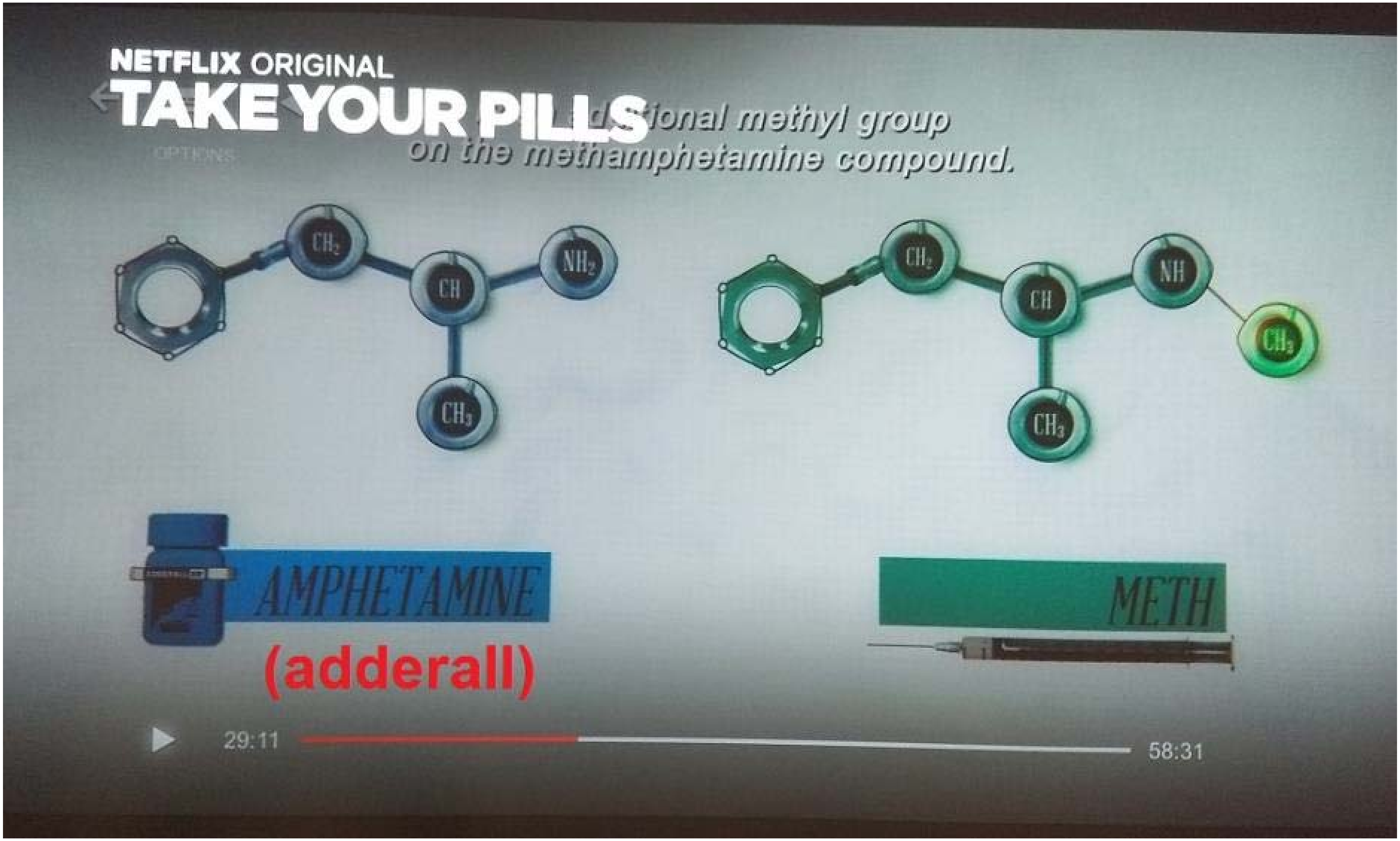


Codeine

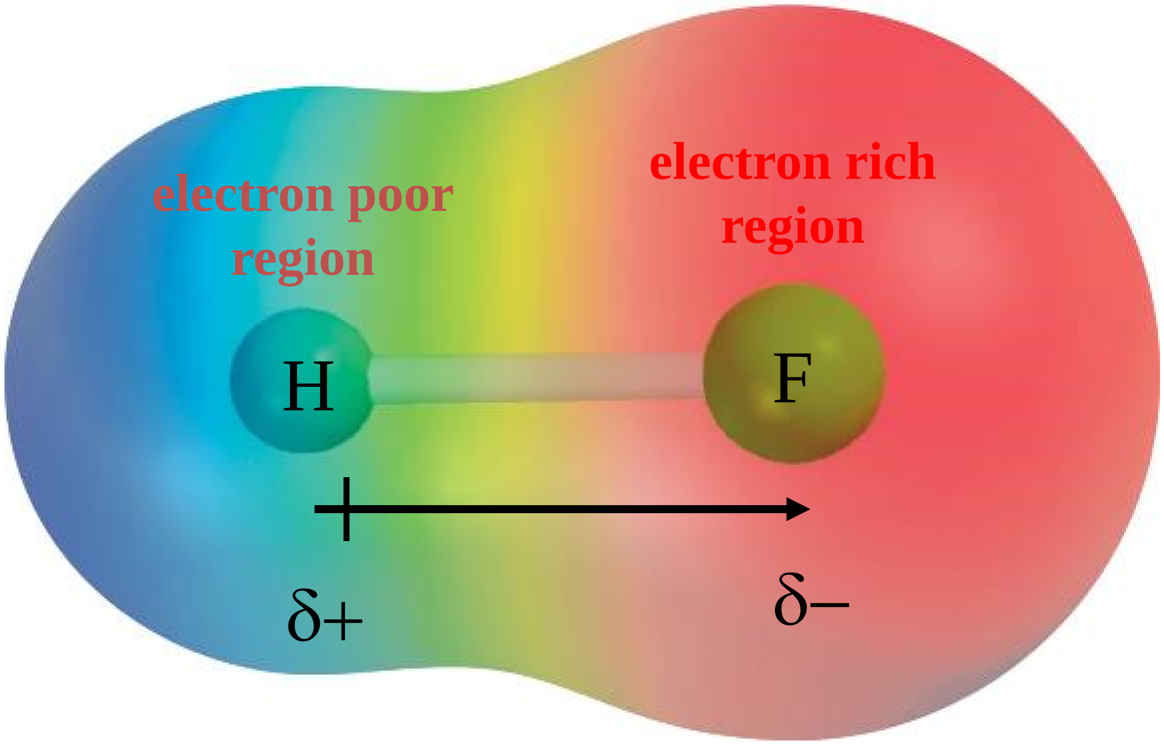


Need to take ~35mg to have the same effect as 5mg of oxycodone

STRUCTURE DETERMINES FUNCTION



POLAR BONDS REVISITED



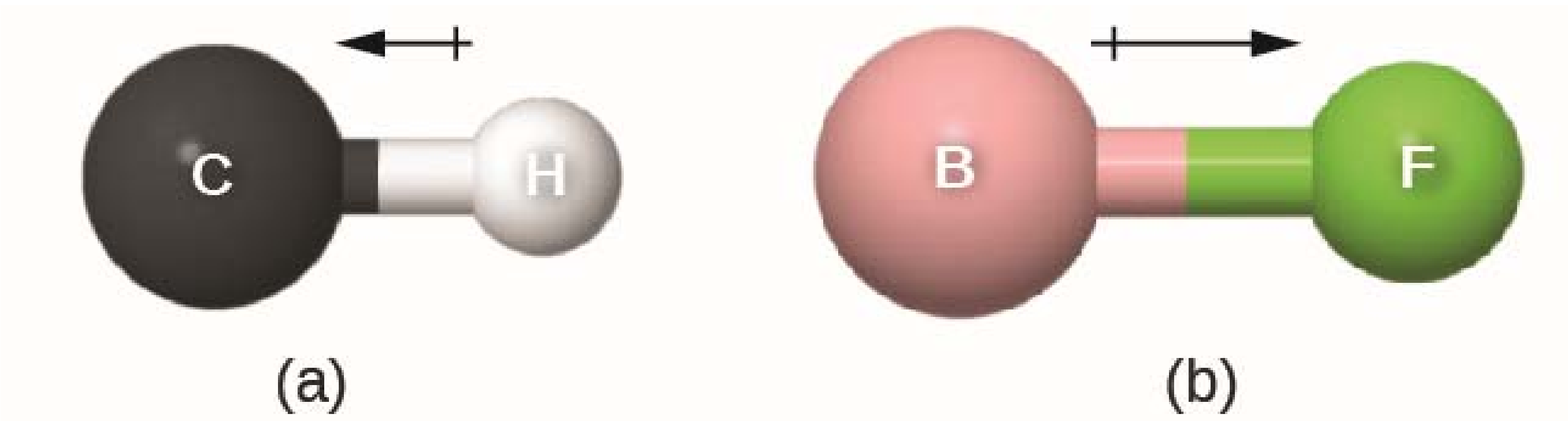
$\mu = Q * r$

Q is the charge

r is the distance between charges

1 D = 3.36×10^{-30} C m

FIGURE 7.26



(a) There is a small difference in electronegativity between C and H, represented as a short vector.

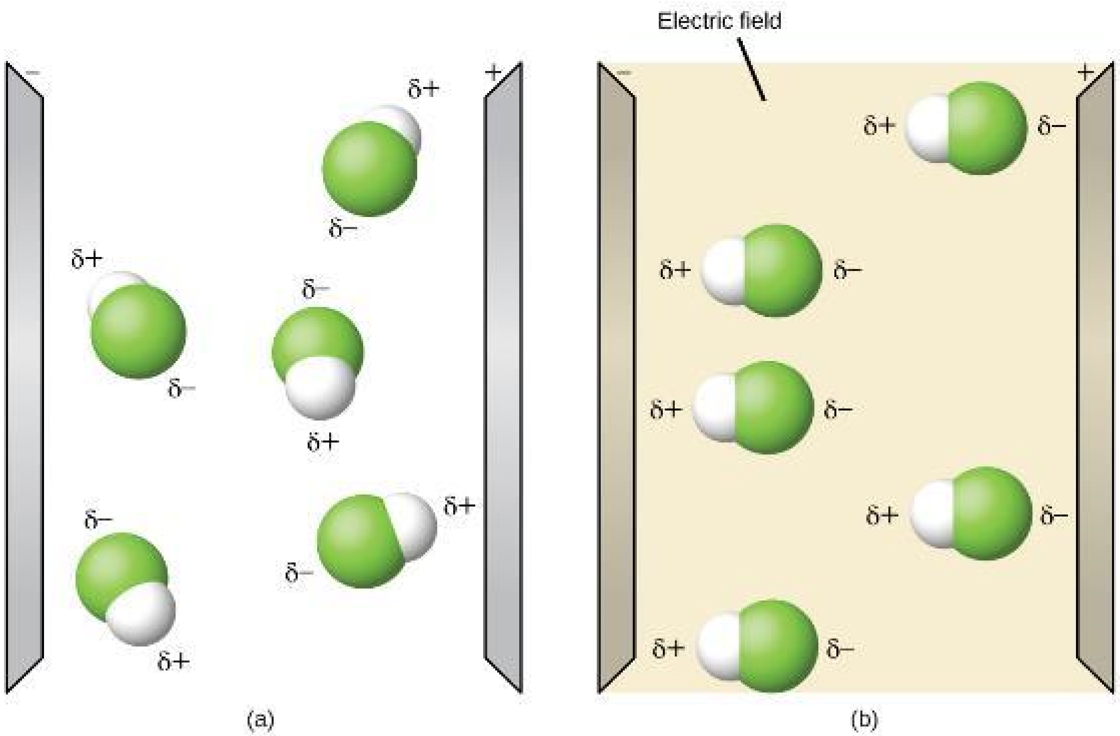
(b) The electronegativity difference between B and F is much larger, so the vector representing the bond moment is much longer.

POLAR MOLECULES

A molecule can have polar bonds (if the bonded atoms have different electronegativities), but it may not possess a dipole moment if it has a highly symmetrical geometry.

Molecule	Geometry	Dipole Moment (D)
HF	Linear	1.92
HCl	Linear	1.08
HBr	Linear	0.78
HI	Linear	0.38
H_2O	Bent	1.87
H_2S	Bent	1.10
NH_3	Trigonal pyramidal	1.46
SO_2	Bent	1.60

BEHAVIOR OF POLAR MOLECULES

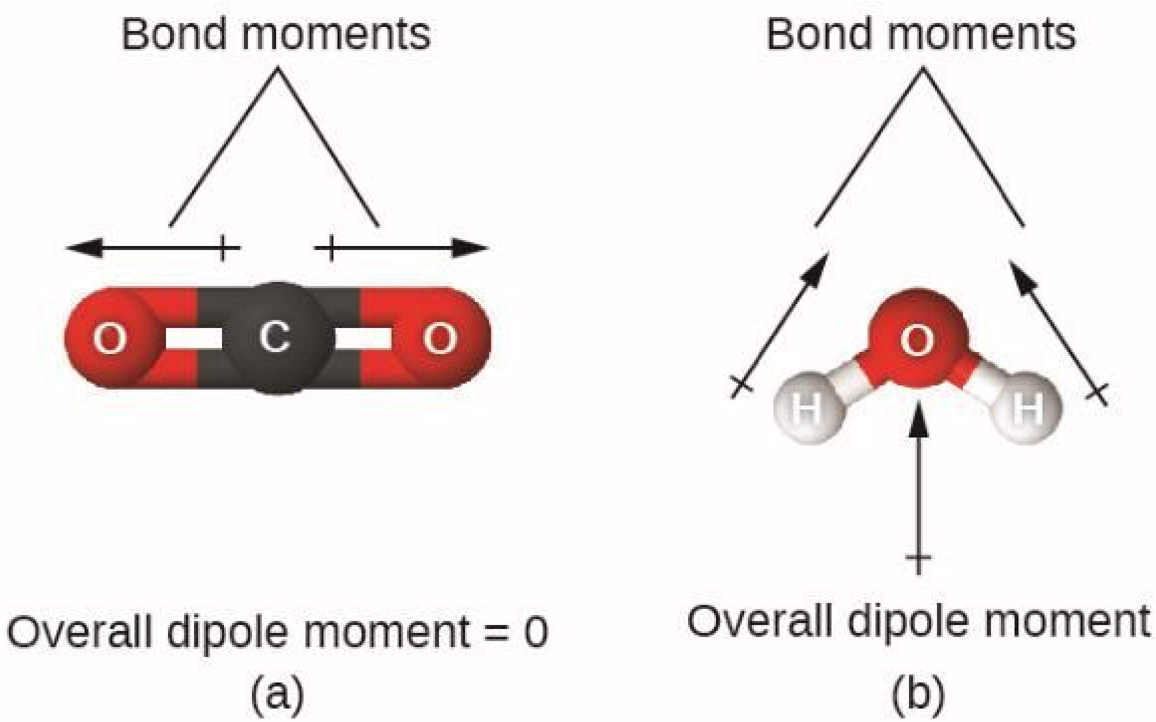


field off field on

(a) Molecules are always randomly distributed in the liquid state in the absence of an electric field.

(b) When an electric field is applied, polar molecules like HF will align to the dipoles with the field direction.

FIGURE 7.27

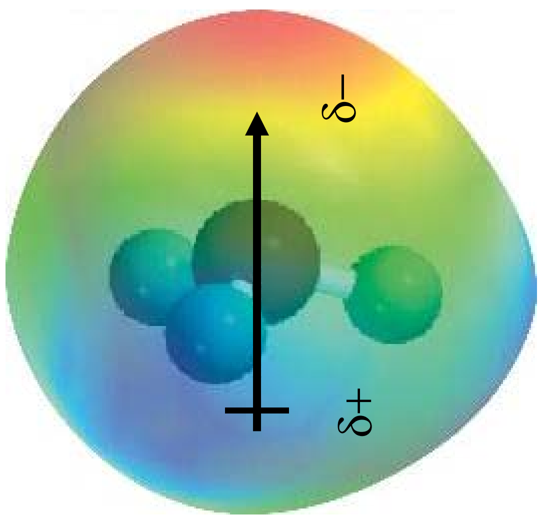


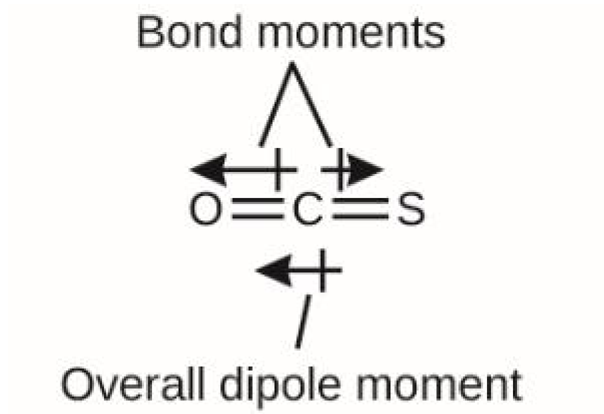
The overall dipole moment of a molecule depends on the individual bond dipole moments and how they are arranged.

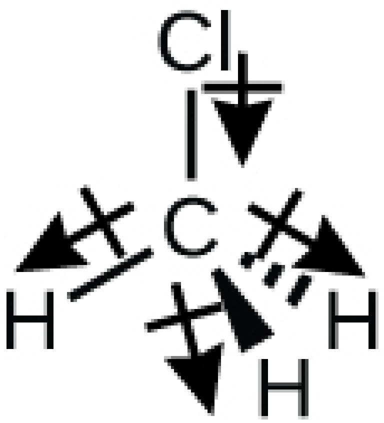
(a) Each CO bond has a bond dipole moment, but they point in opposite directions so that the net CO_2 molecule is nonpolar.

(b) In contrast, water is polar because the OH bond moments do not cancel out.

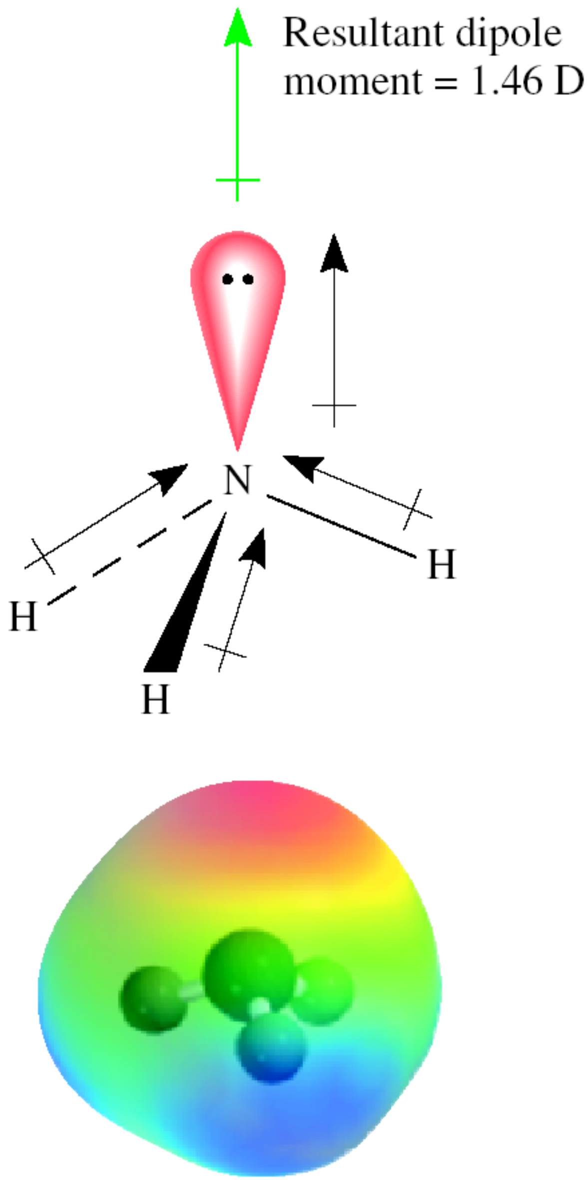
MORE EXAMPLES

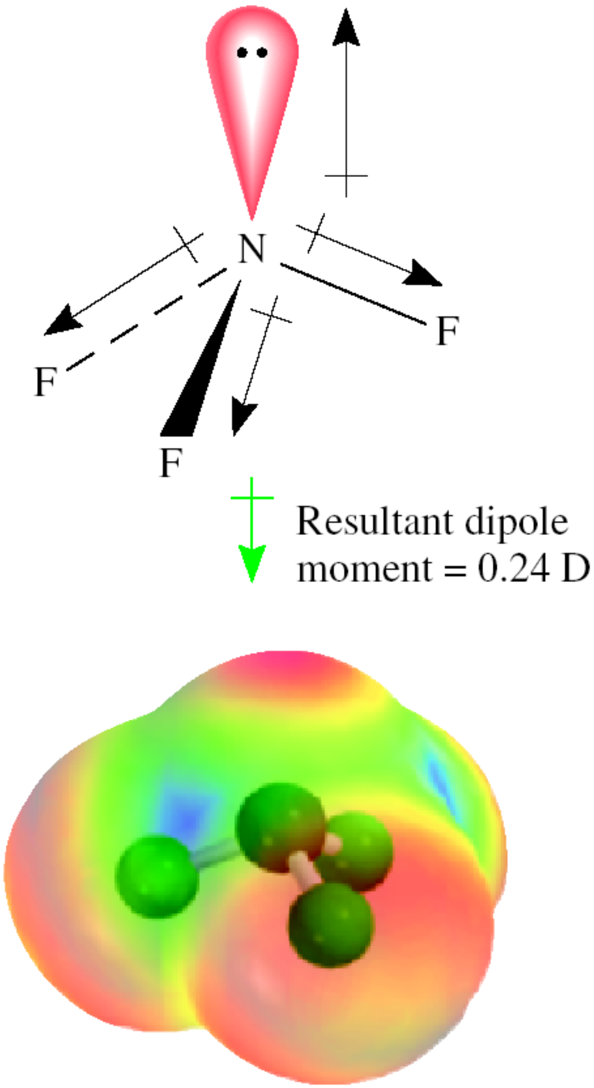




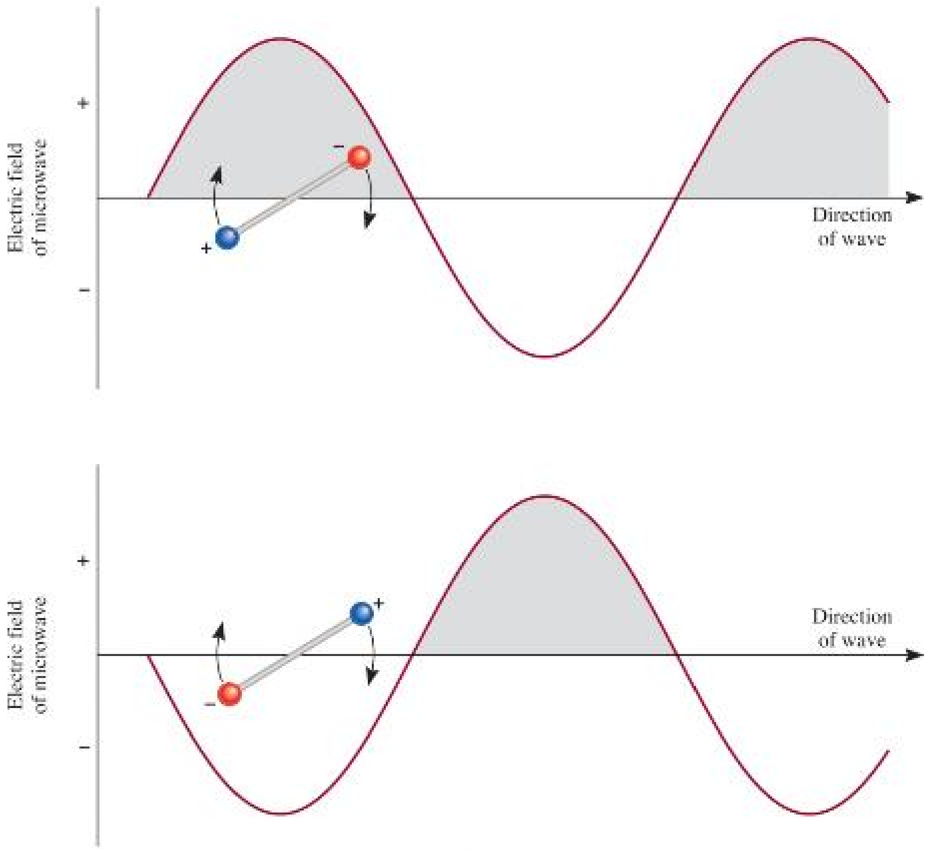


NH_3 AND NF_3

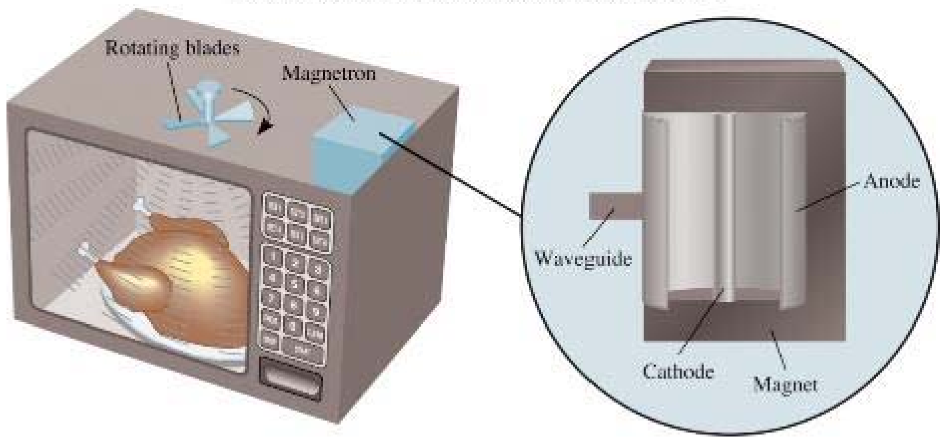

Resultant dipole
moment = 1.46 D
N
H
H
H


N
F
F
F
Resultant dipole
moment = 0.24 D

MICROWAVE OVENS



(b)



QUESTION

Predict whether each of the following molecules has a dipole moment:

(a) BrCl

(b) BF_3 (trigonal planar)

(c) CH_2Cl_2 (tetrahedral)

HW problems:

5, 8, 13, 17, 21, 25, 30, 35, 45, 47, 52, 58, 65, 70, 75, 81, 89, 93, 99, 105, 116