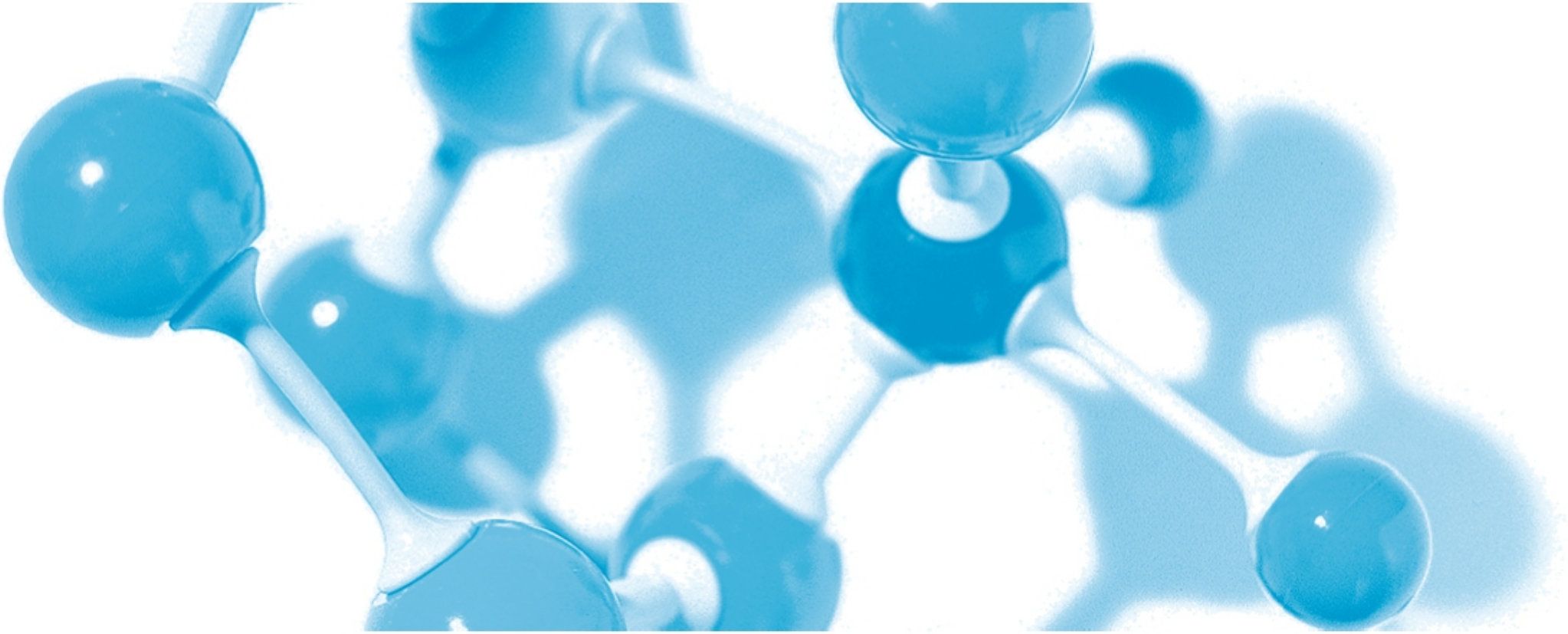


Bonding – Chapter 7

Bond – an attractive force that holds two atoms together.

Atoms bond to obtain a more stable electronic configuration.

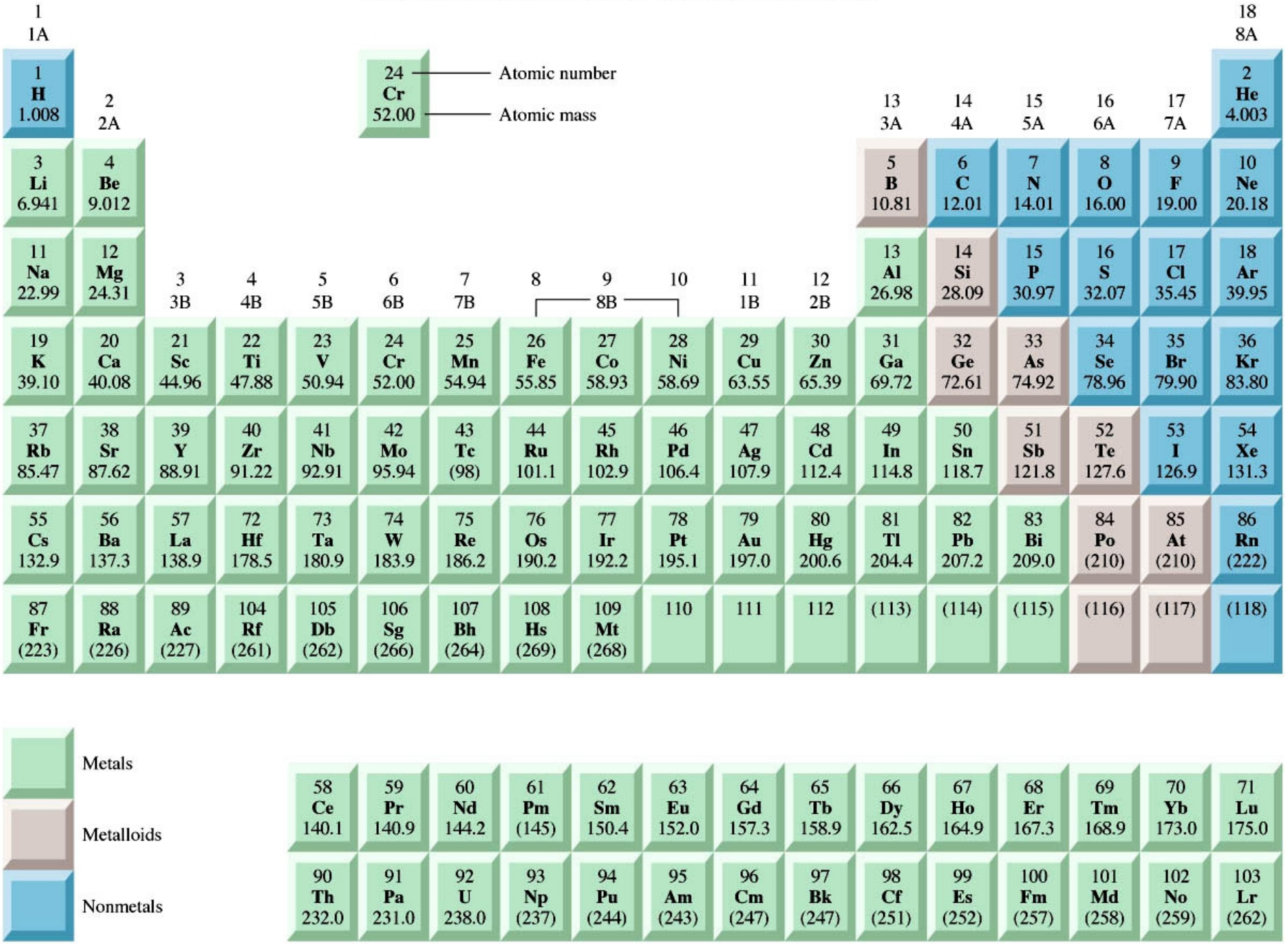
- Ionic bonds – attraction between oppositely charged atoms/molecules
- Covalent bonds – atoms tied together by sharing electrons
- Metallic bonds – metallic atoms all sharing outer electrons in a 'sea of electrons'

- Only outer electrons participate in bonding
  - Inner electrons are in stable Noble Gas configurations
- Valence Shell – outermost occupied ground state shell
- Valence electrons (v.e.) – electrons in valence shell

Valence electrons (ve)

- The outer electrons are called “valence electrons” or “bonding electrons”
- Most atoms want to get 8 v.e. (octet rule), which they do by gaining, losing, or sharing electrons.
  - Main exception: Hydrogen wants 2 v.e.
- Noble gases already have 8 v.e. (except helium which has 2), which is why they almost never react.

Group	Valence electrons
1 (1A)	1
2 (2A)	2
13 (3A)	3
14 (4A)	4
15 (5A)	5
16 (6A)	6
17 (7A)	7
18 (8A)	8 (He has 2)



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He: $1s^2$

Ne: $1s^2 2s^2 2p^6$

Ar: $1s^2 2s^2 2p^6 3s^2 3p^6$

Kr: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$

Xe: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6$

Rn: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6$

Ions

- Cations – lost one or more electrons
  - positively charged

- Anions – gained one or more electrons
  - negatively charged

- When forming ions, atoms usually want to get to the same number of electrons as the nearest Noble Gas

Group	Ion usually formed
1 (1A)	+1 H can form -1 ion
2 (2A)	+2
13 (3A)	+3
14 (4A)	+/-4
15 (5A)	-3
16 (6A)	-2
17 (7A)	-1
18 (8A)	0

Isoelectronic species

- Atoms/ions with the same electronic configuration

- Will have the same number of electrons, but:
  - different numbers of protons
  - different charges

K^{+1}, Ar, and Cl^{-1} are all isoelectronic

TABLE 7.1 Ions Isoelectronic with Selected Noble Gases

Electron Configuration	Anions			Noble Gas	Cations		
$1s^2$			H^-	He	Li^+	Be^{2+}	
$1s^2 2s^2 2p^6$	N^{3-}	O^{2-}	F^-	Ne	Na^+	Mg^{2+}	Al^{3+}
$1s^2 2s^2 2p^6 3s^2 3p^6$	P^{3-}	S^{2-}	Cl^-	Ar	K^+	Ca^{2+}	Sc^{3+}

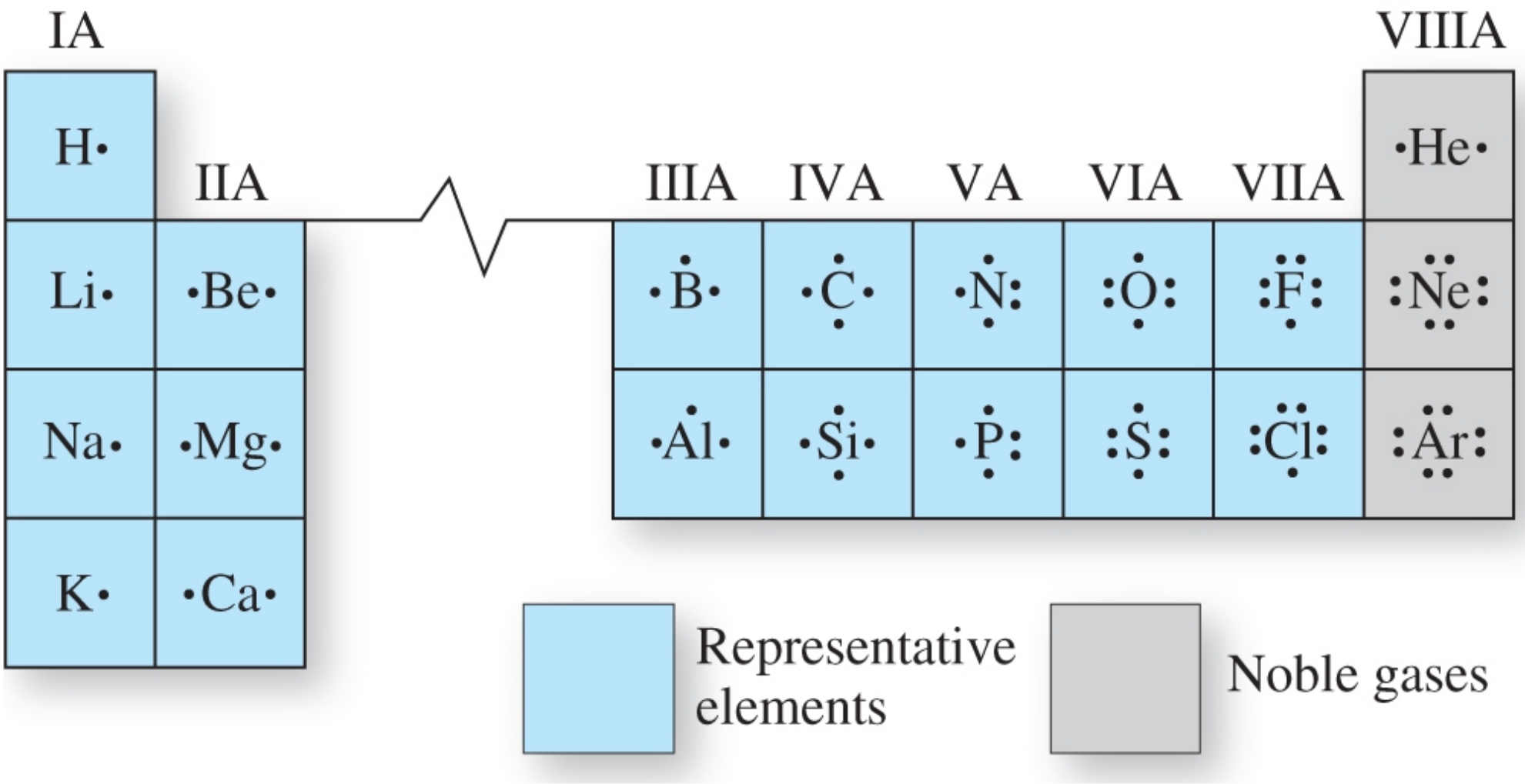
Ionic Radii

- When an atom:
  - gains an electron, the radius increases
  - loses an electron, the radius decreases
- Therefore:
  - Cations have smaller radii than the parent atom
  - Anions have larger radii than the parent atom

- For isoelectronic species (same # of electrons):
  - Larger nuclear charges pull harder on the e^-
  - Therefore, the larger the atomic number, the smaller the radius

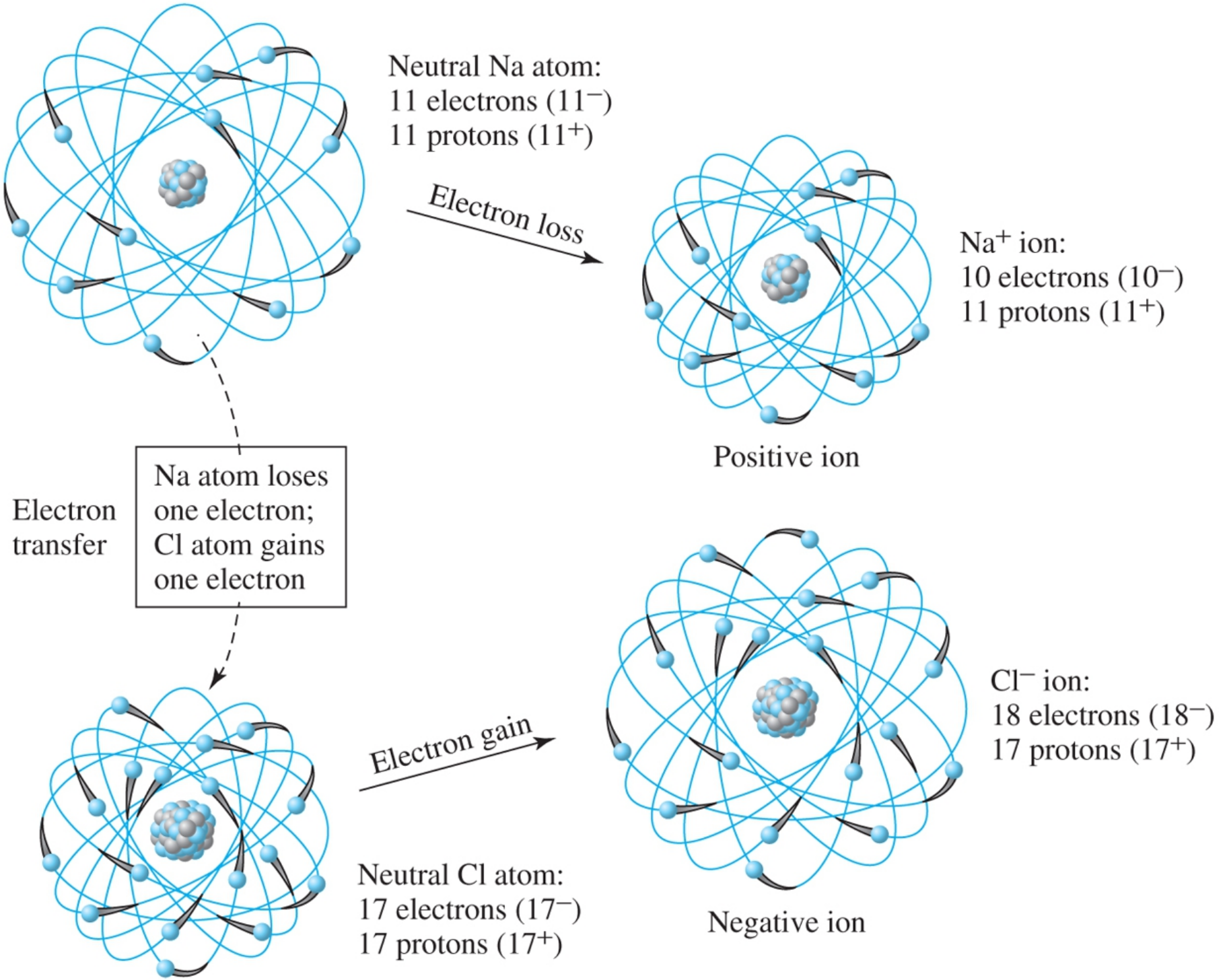
Lewis Structures

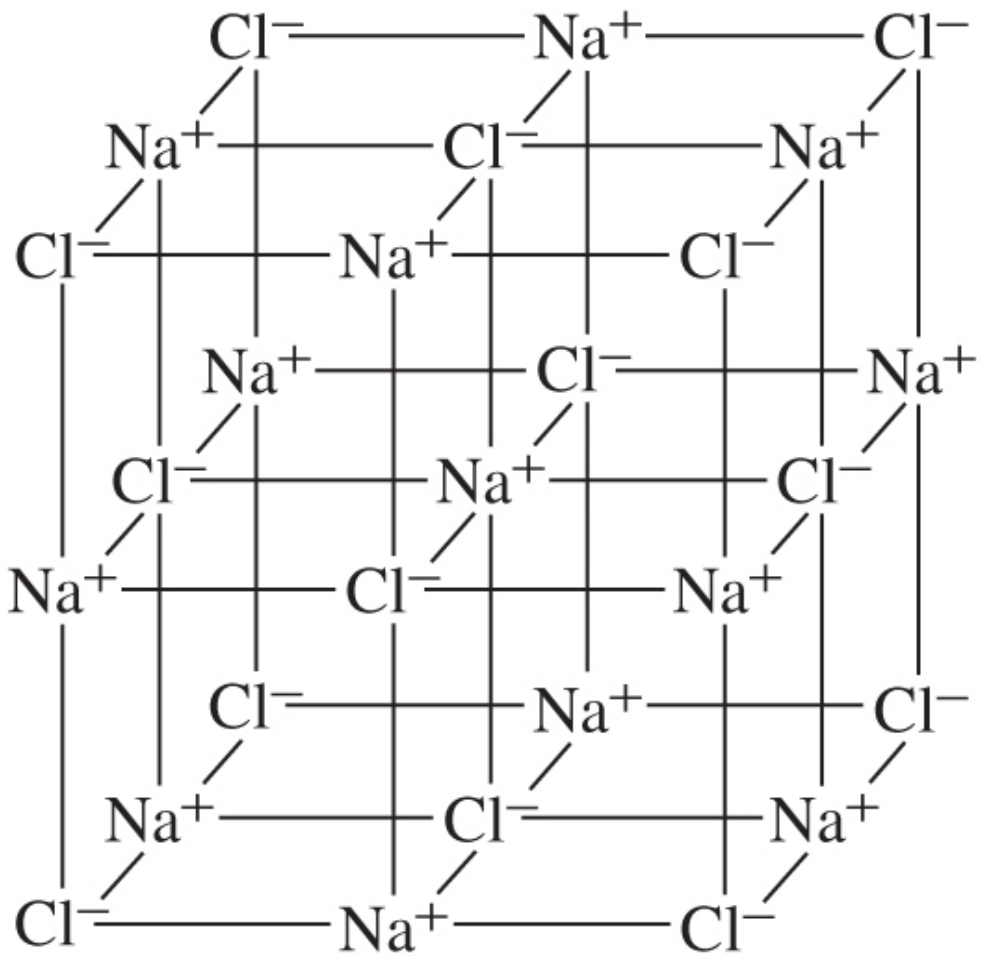
- Use chemical symbols and valence electrons to show bonding
  - Used to predict chemical structures
  - Used to predict molecular geometries
  - This information is used to predict chemical and physical properties

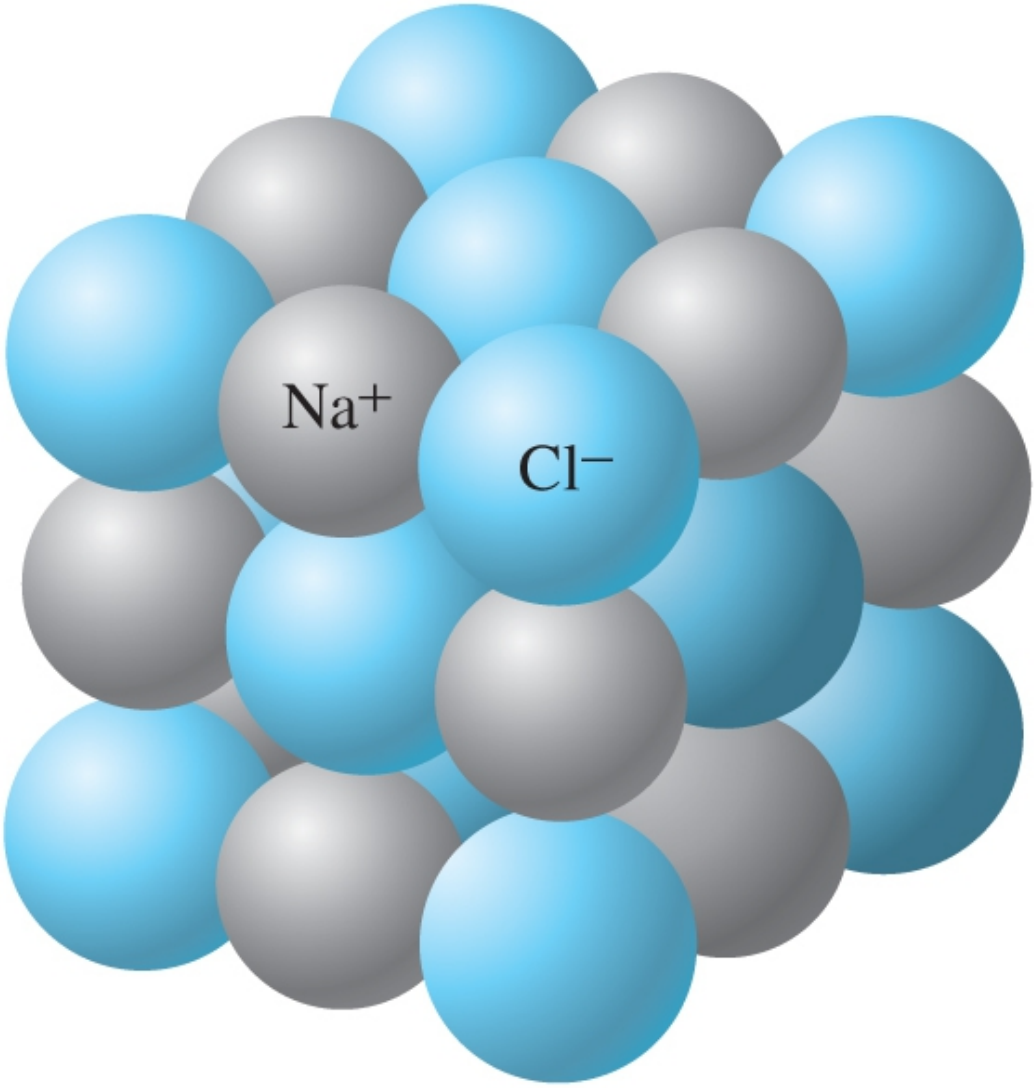


Ionic Compounds (form between metals and non-metals)

- Electrically neutral overall
- Anions are attracted to all nearby cations
  - Larger charge – stronger attraction
  - closer proximity – stronger attraction
- All nearby opposite charges attract each other
- All nearby similar charges repel each other
- Solids form crystalline structures
  - ordered to maximize attraction, minimize repulsion







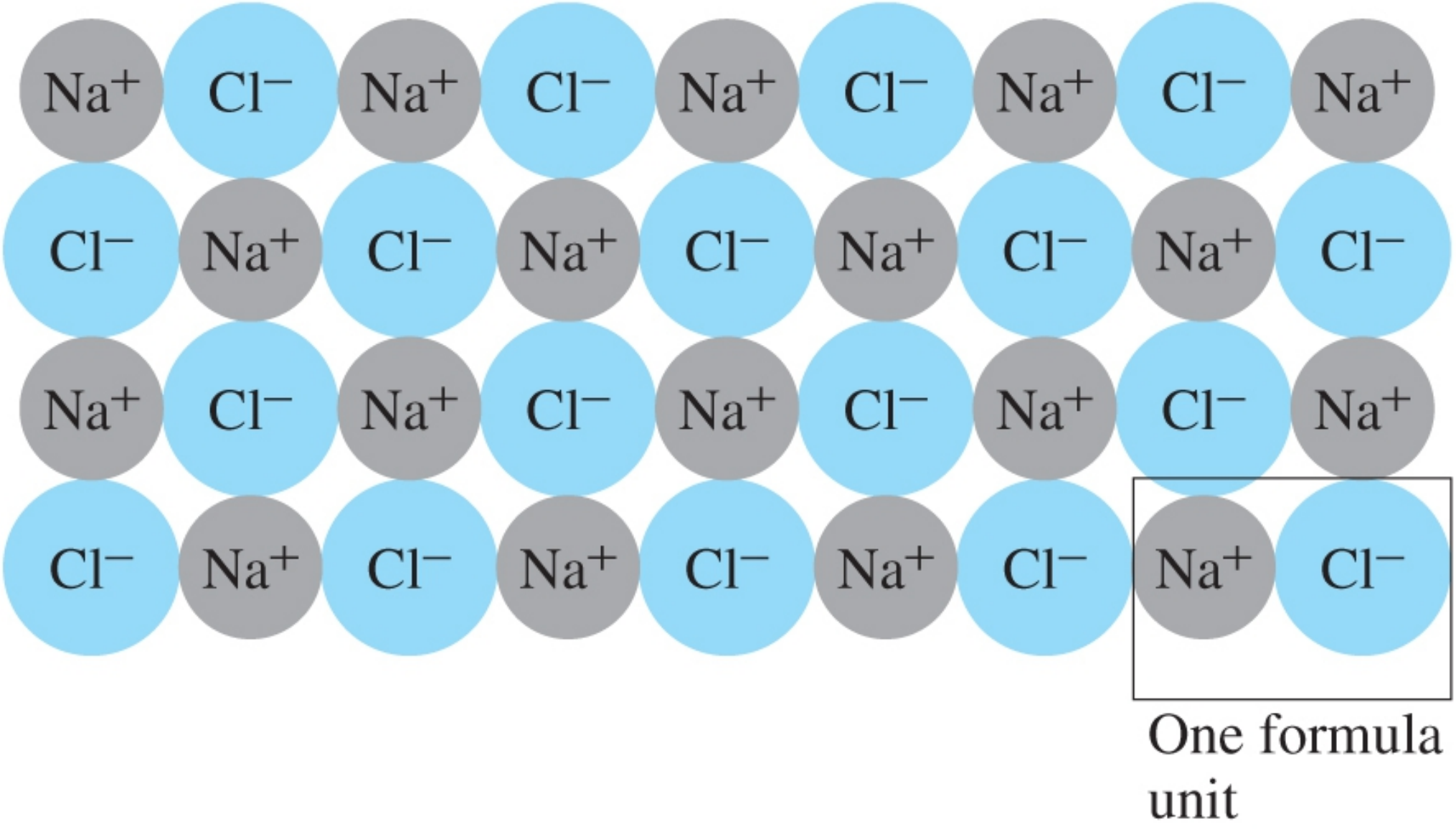
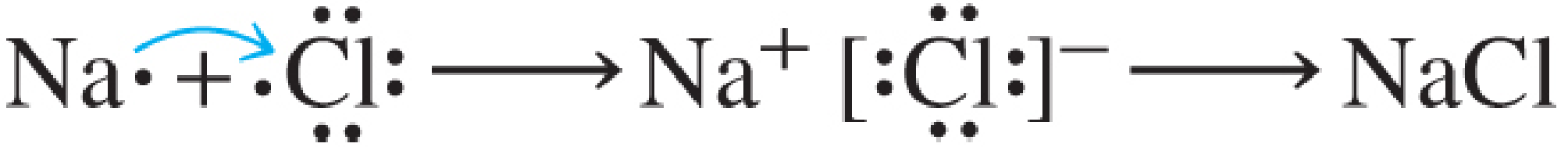
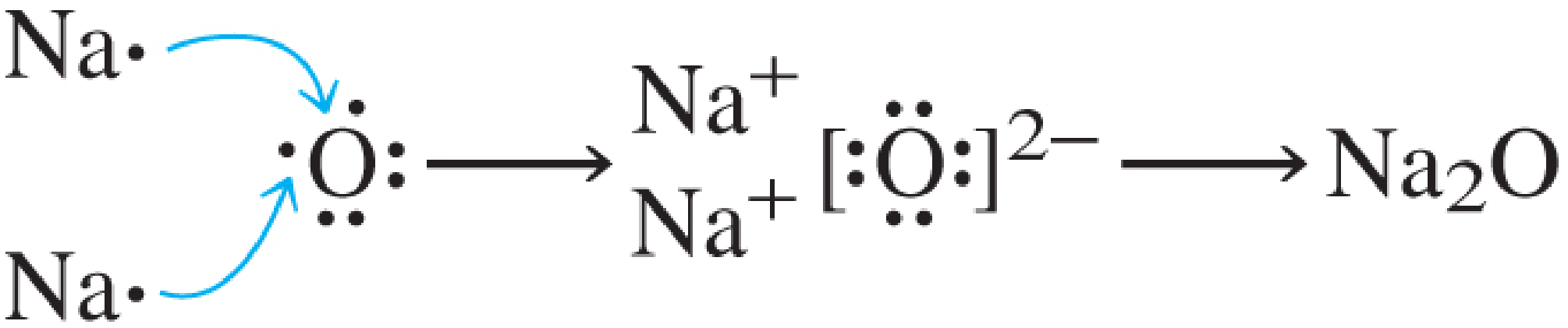
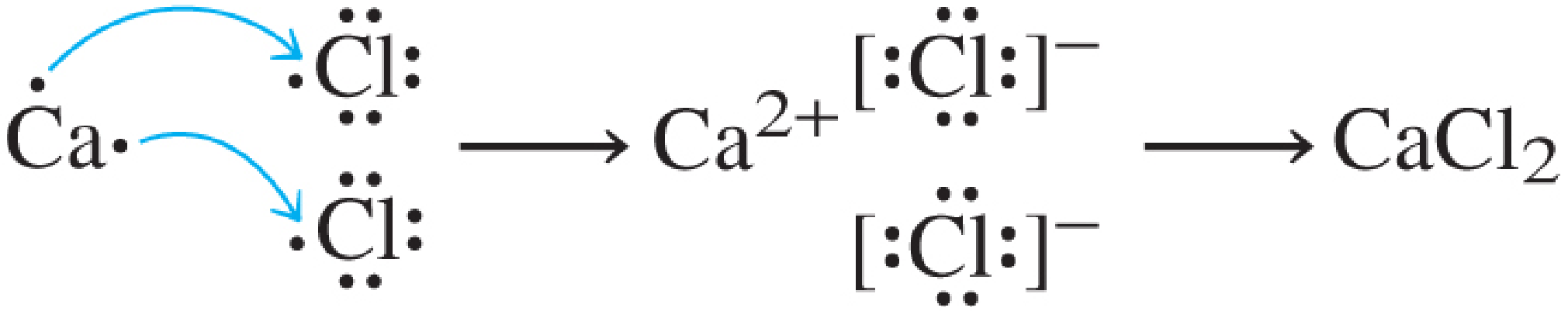


TABLE 7.3 General Formulas for Ionic Compounds as a Function of Periodic Table Position of the Metal and Nonmetal

	Nonmetals (X)		
Metals (M)	**VIIA (−1 ions)**	**VIA (−2 ions)**	**VA (−3 ions)**
IA (+1 ions)	MX	M_2X	M_3X
IIA (+2 ions)	MX_2	MX	M_3X_2
IIIA (+3 ions)	MX_3	M_2X_3	MX

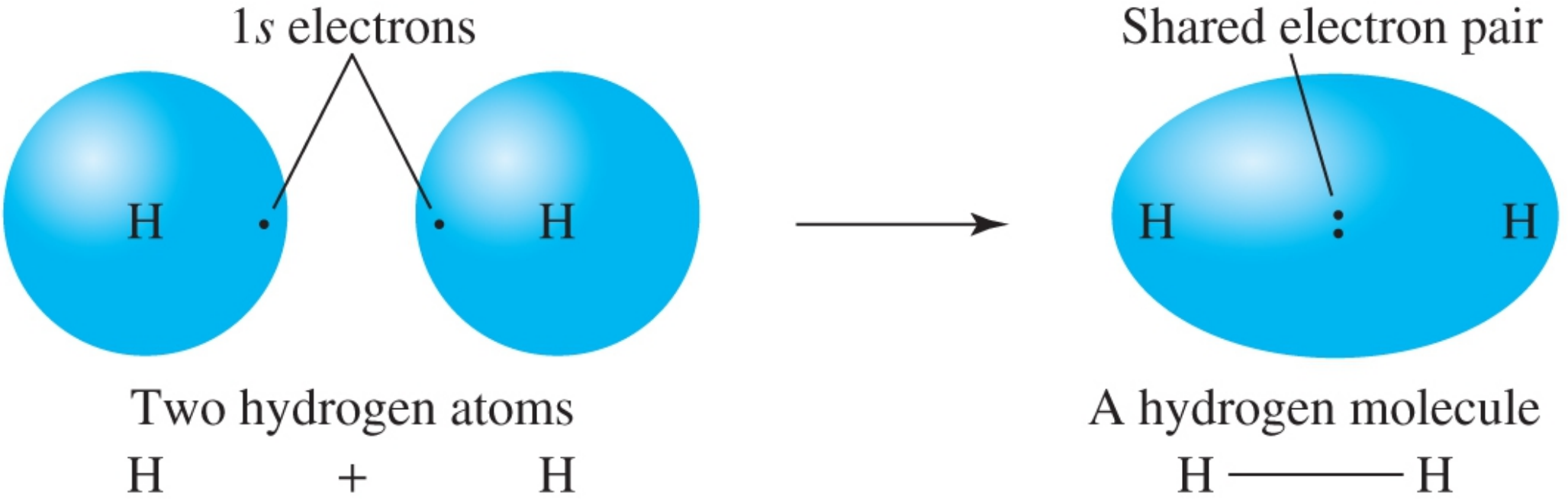


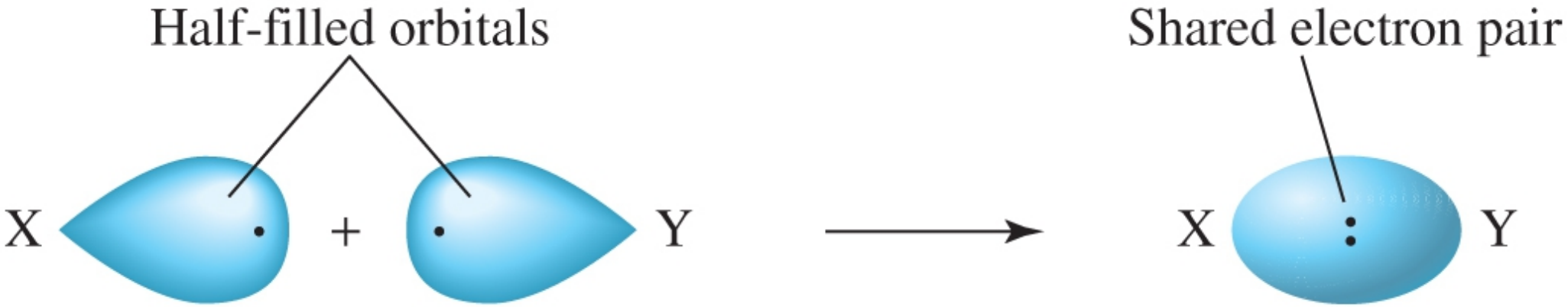




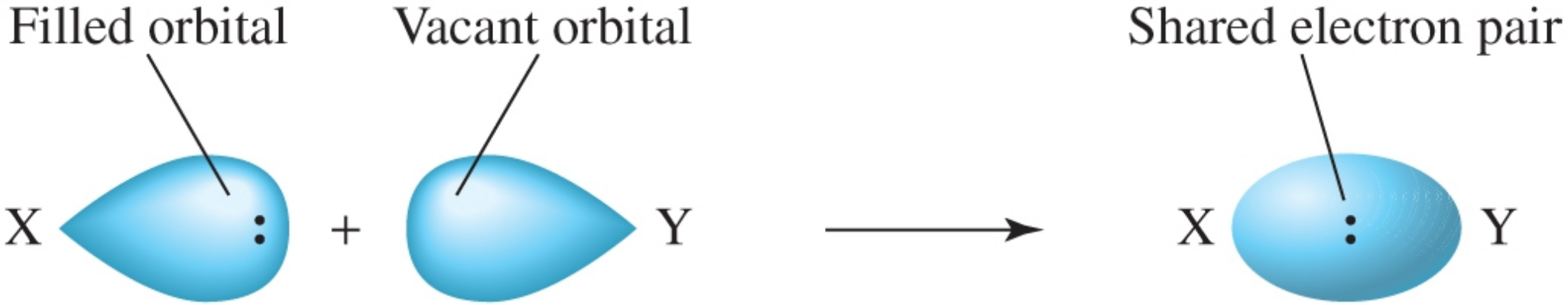
Covalent Bonds

- Occurs between non-metals and non-metals
- Shared electrons 'tie' atoms together
- Shared electrons count toward valence electrons of both atoms
  - single bond = two shared e^-
  - double bond = four shared e^-
  - triple bond = 6 shared e^-

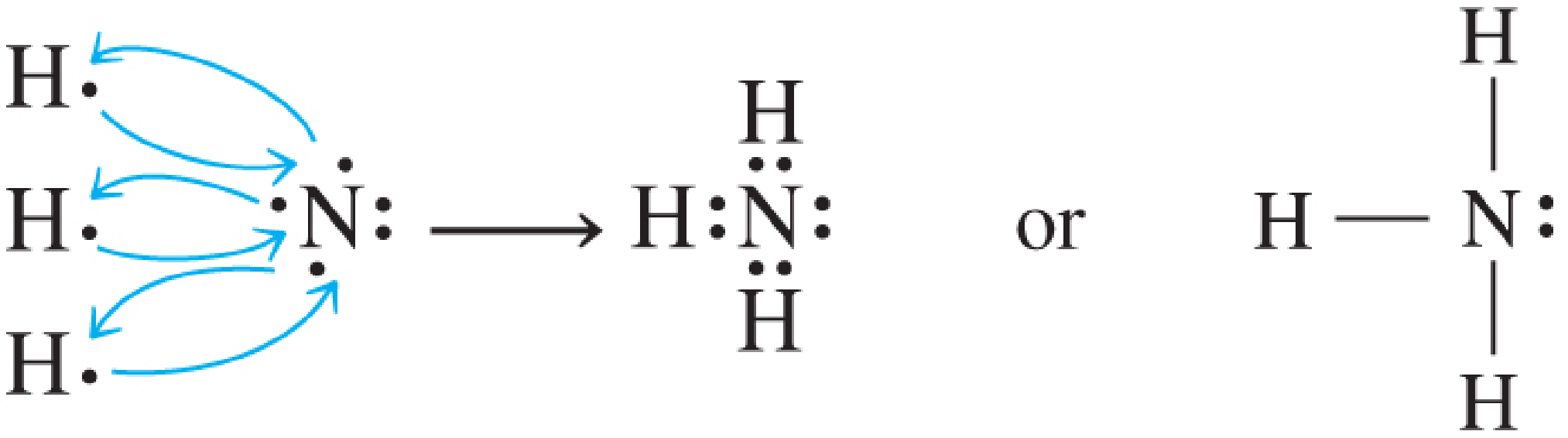


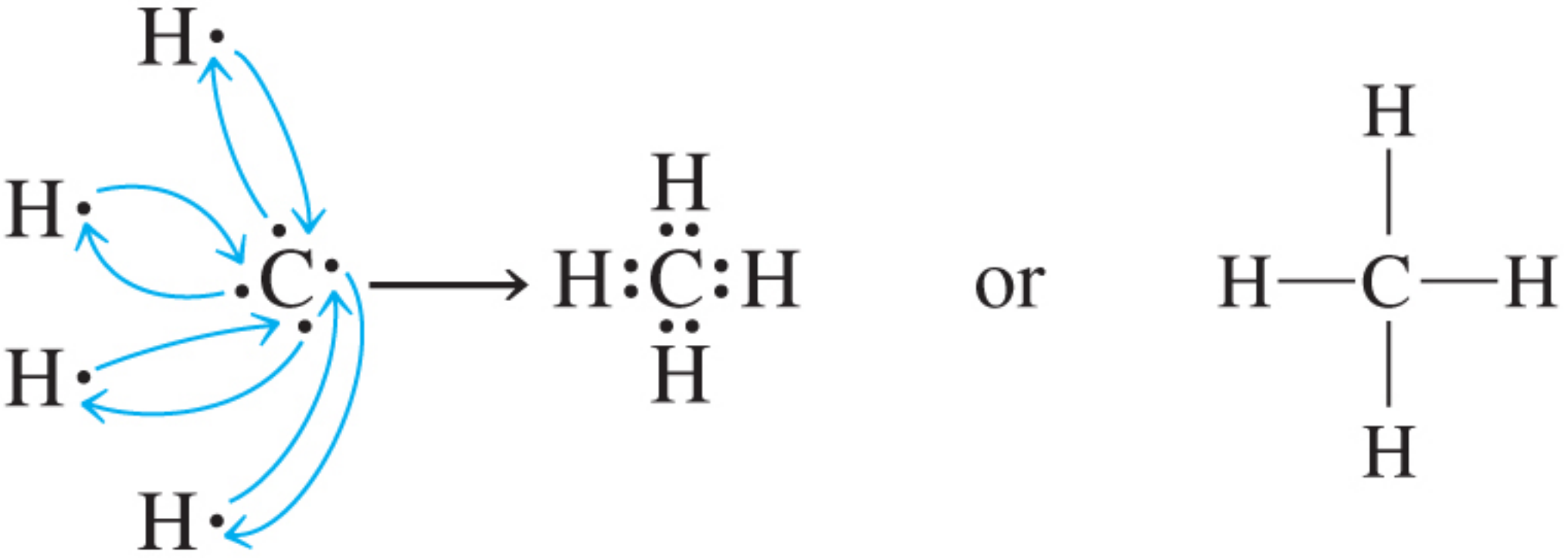


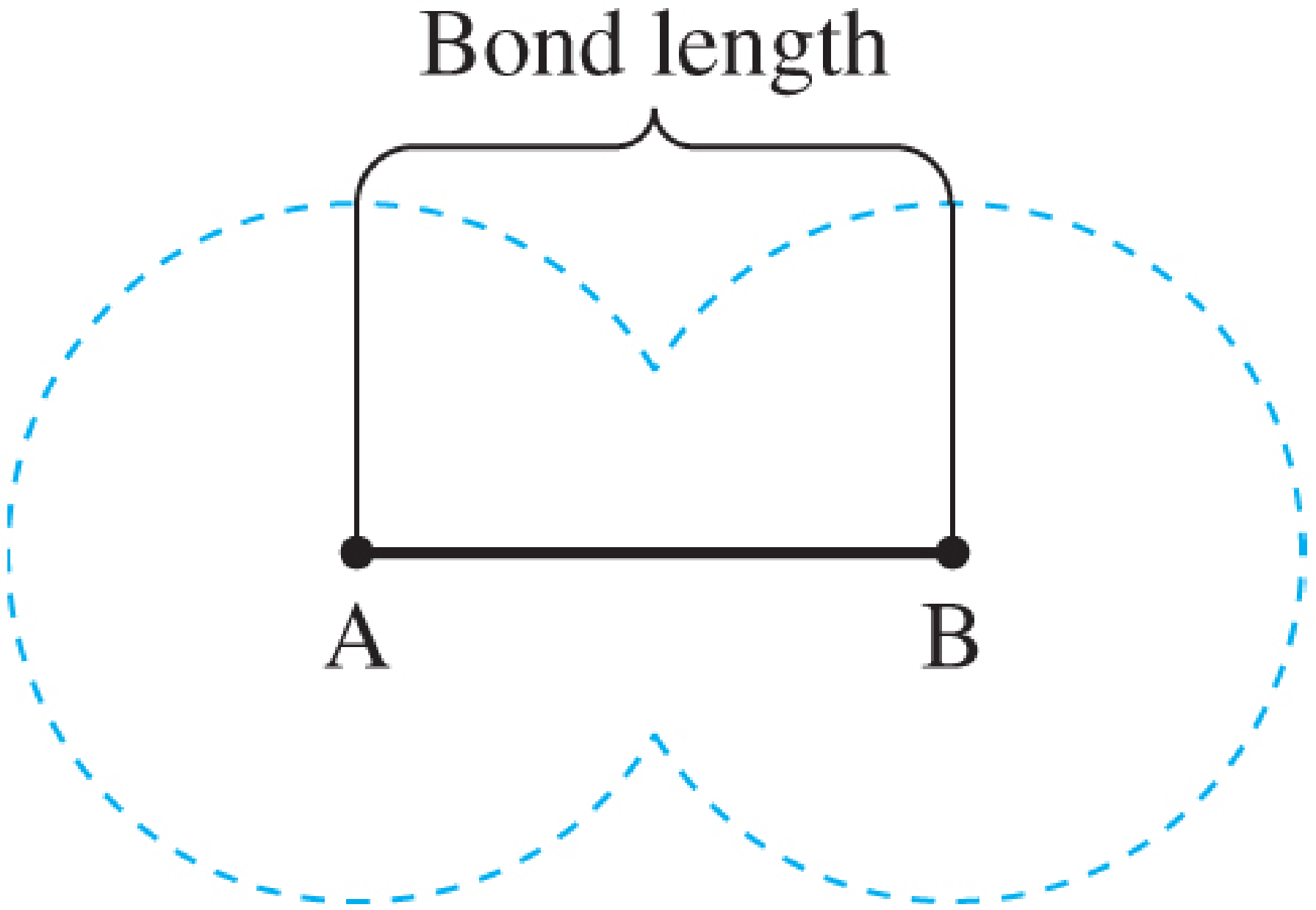
(a) Regular covalent single bond



(b) Coordinate covalent single bond



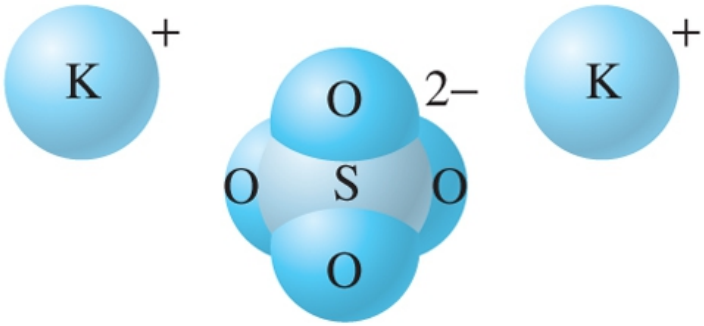
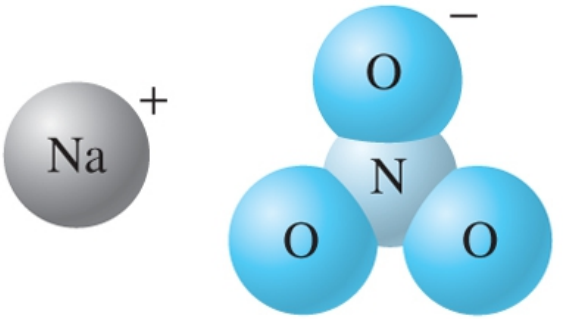
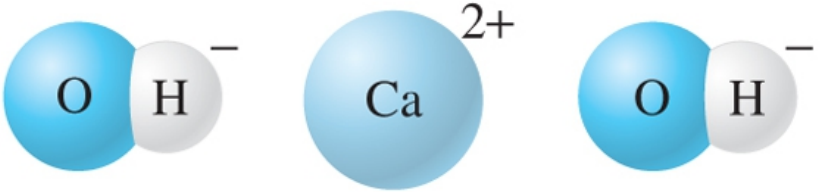




Polyatomic ions

Molecules (covalently bonded atoms) with an overall negative or positive charge.

NO_3^{-1}	Nitrate ion
SO_4^{-2}	Sulfate ion
OH^{-1}	Hydroxide ion
NH_4^{+1}	Ammonium ion
(NH_3	Ammonia, not an ion)
CO_3^{-2}	Carbonate
PO_4^{-3}	Phosphate
ClO_3^{-1}	Chlorate
H_3O^{+1}	Hydronium ion

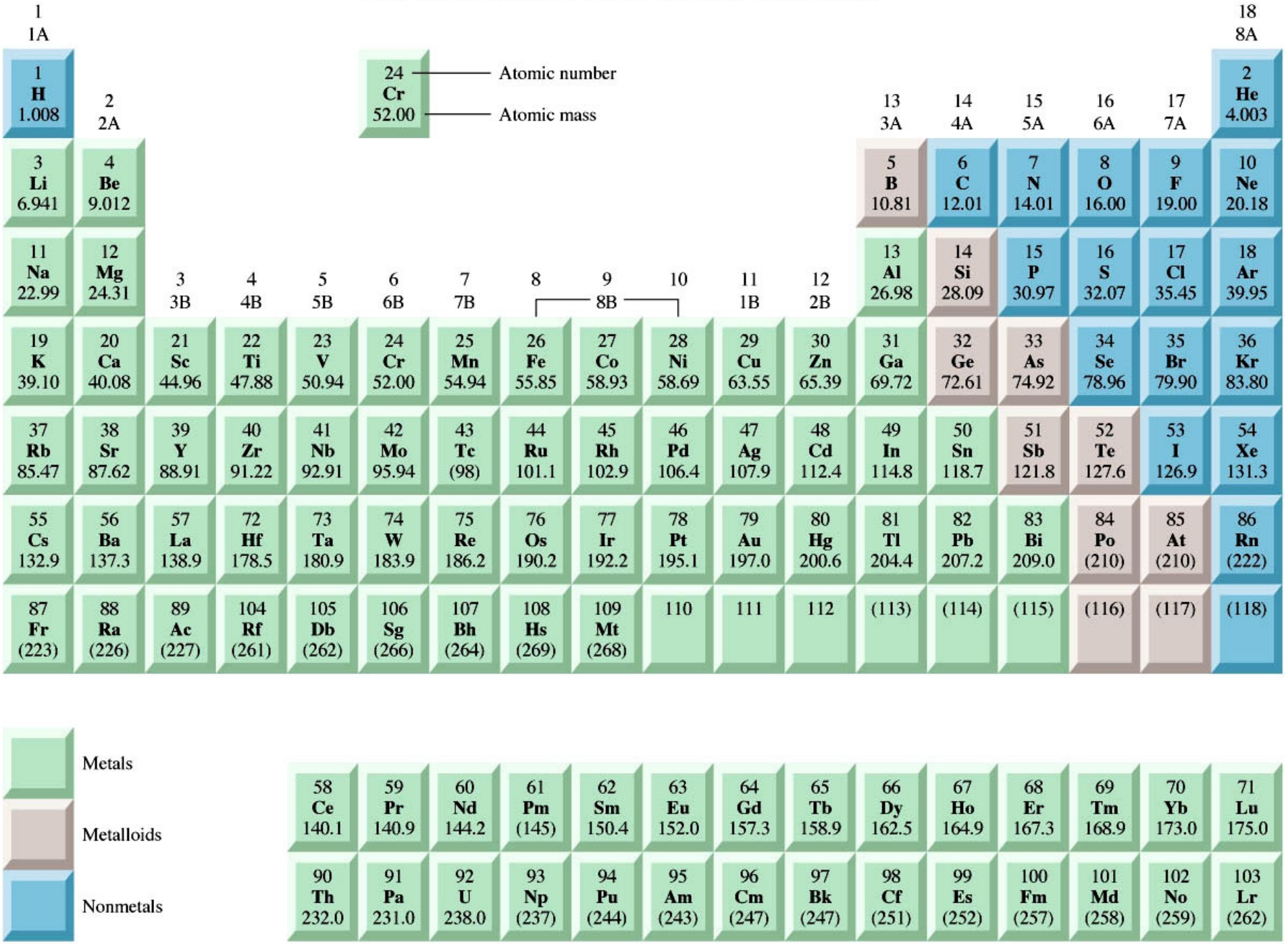
K_2SO_4 Potassium sulfate	
$NaNO_3$ Sodium nitrate	
$Ca(OH)_2$ Calcium hydroxide	
NH_4CN Ammonium cyanide	

To draw Lewis Structures for molecules:

- Add up valence electrons for all atoms
- Draw backbone ('skeletal structure') for the molecule
  - Link atoms with single bonds (two shared electrons)
  - Usually elements down and to left on PT are central (carbon is usually central)
  - H and Group 17 elements almost always only form single bonds

- Add electrons to satisfy the octet rule for all atoms:
  - Add electrons to outer atoms first
  - Electrons usually placed in pairs above, below, right, or left of symbol
  - Electrons between two atoms are bonding electrons, and count toward valence electrons for both atoms
    - 2 shared e^- - one line – single bond
    - 4 shared e^- - two lines – double bond
    - 6 shared e^- - three lines – triple bond

- Use/move unshared pairs of electrons to form double and triple bonds, if needed, to satisfy octets
- Double check:
  - Final structure must have the exact number of total valence electrons
  - Check that all atoms obey the octet rule, not counting the few exceptions
  - [(sum of desired v.e. over all atoms) – (total valence electrons)]/2 = total # of bonds



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- Following the above procedure may result in several different Lewis Structures being drawn

- Formal Charges will often show which is the more stable, preferred, structure

- Formal charges for each atom should add up to the overall charge for the atom/molecule

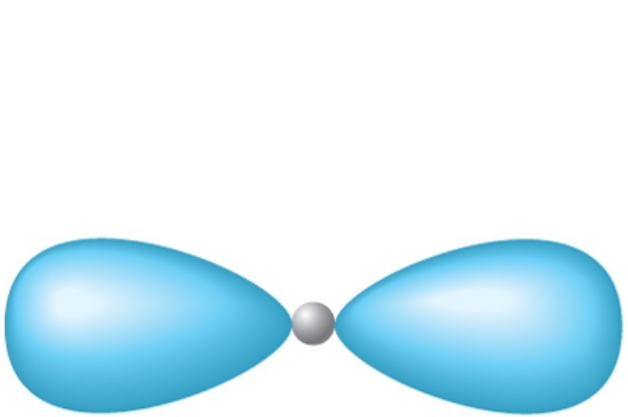
- Formal charge (FC) shows the effective charge on each atom
- FC = valence electrons – unshared electrons – 1/2 bonding electrons
- FC = v.e. – u.e. – 1/2 b.e.
- Structures with FCs closer to 0 are preferred
- Negative FCs should be on more electronegative atoms

- Not all molecules can be accurately represented by a single Lewis Structures
  - Sometimes two or more structures may be drawn with identical formal charges
  - In this case the actual structure of the molecule is an average of all of the similar structures
- These are called Resonance Structures

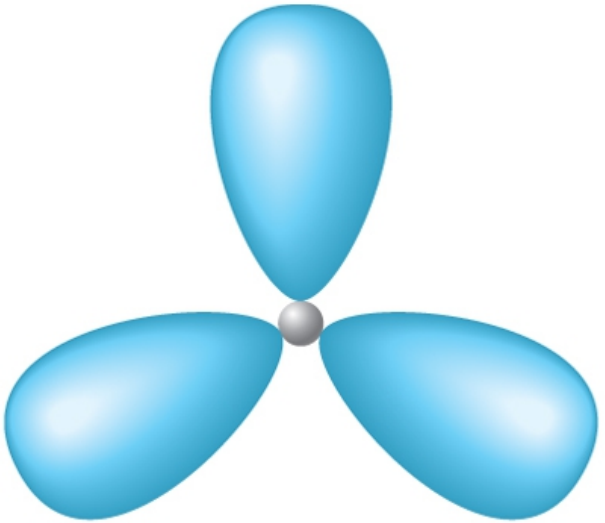
Molecular Geometry

- The geometric shape of a molecule may be determined from the Lewis Structure
- Groups of valence electrons on an atom repel each other, and move to maximize their angles of separation
- Groups of electrons are:
  - Unshared pairs of electrons
  - single bonds
  - double bonds
  - triple bonds

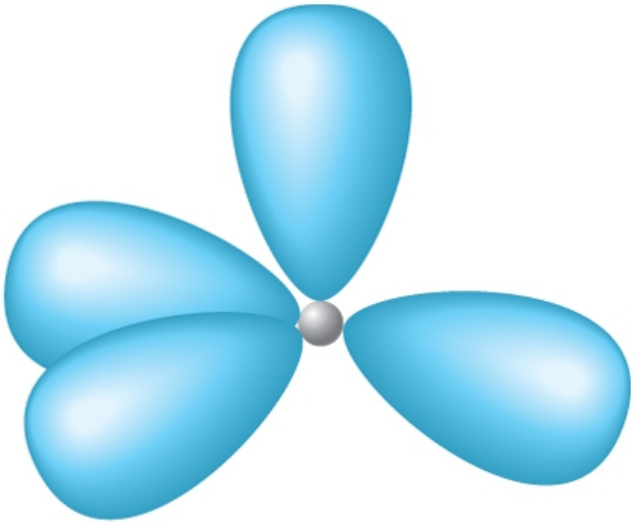
- With two groups – 180° between groups
  - Linear
- With three groups – 120° between groups
  - Trigonal
- With four groups – 109.5° between groups
  - Tetrahedral
- The actual shape of the molecule is dependent on the actual bonds.



Two balloons, linear



Three balloons, trigonal planar

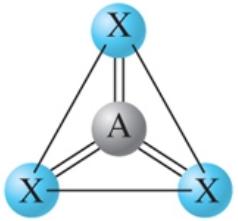
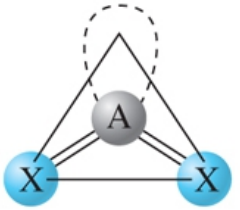


Four balloons, tetrahedral

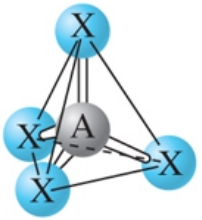
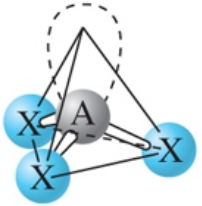
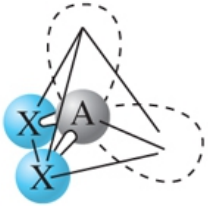
Two VSEPR Electron Groups

Two double bonds	One triple bond and one single bond
	
Linear	Linear
CO_2	HCN

Three VSEPR Electron Groups

One double bond and two single bonds	One double bond, one single bond, and one nonbonding pair
	
Trigonal planar	Angular or bent
H_2CO, $COCl_2$	SO_2, S_2O

Four VSEPR Electron Groups

Four single bonds	Three single bonds and one nonbonding pair	Two single bonds and two nonbonding pairs
		
Tetrahedral	Trigonal pyramidal	Angular or bent
CH_4, $SiCl_4$	NH_3, PF_3	H_2O, OF_2

Note: The figure does not consider cases where only one bond is present—for example, one single bond and three nonbonding pairs. If only one bond is present, the molecule is diatomic. All diatomic molecules have the same geometry: The two atoms lie along a straight line.

- Electronic Geometry
  - Use all groups of electrons to determine the angles between groups

- Molecular Geometry
  - Look only at bonds to determine the shape of the molecule
  - Angles between bonds determined by electronic geometry
  - For central atoms with no unshared electrons, el. geom. = mol. geom.

Molecular Formula	Lewis Structure and VSEPR Electron-Pair Analysis	Molecular Geometry
C_2H_2 (acetylene)	H—C≡C—H Two VSEPR electron groups; linear C center Two VSEPR electron groups; linear C center	H—C≡C—H Straight chain of four atoms—linear
HN_3 (hydrogen azide)	H—N=N=N: Three VSEPR electron groups; angular N center Two VSEPR electron groups; linear N center	N=N=N: H Chain of four atoms with one bend
H_2O_2 (hydrogen peroxide)	H—O—O—H Four VSEPR electron groups; angular O center Four VSEPR electron groups; angular O center	O—O H H Chain of four atoms with two bends

overall molecular geometry. Figure 7.11 shows the results of such procedures for selected molecules containing more than one central atom.

also called:

VSEPR Theory

Valence Shell Electron Pair Repulsion

- Electronegativity (EN) – attraction for bonding (shared) electrons

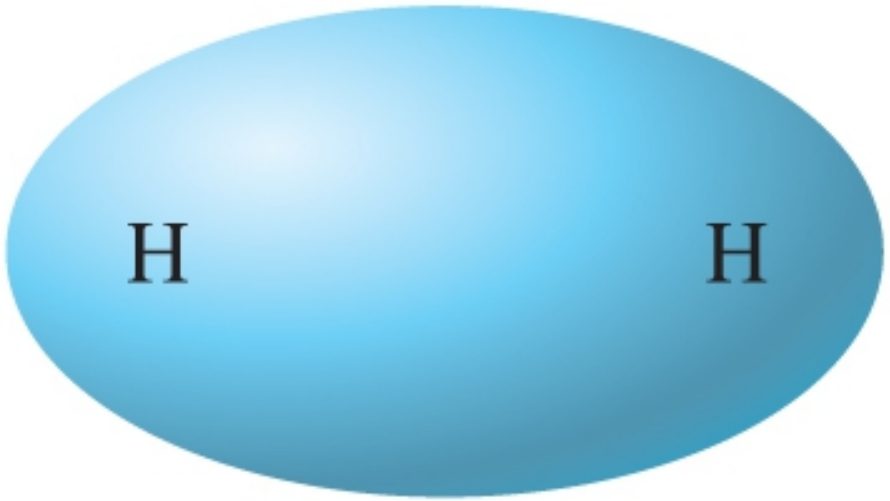
The difference in EN between the bonding atoms determines if the bond is ionic or covalent

H 2.1																	He –
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne –
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar –
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 1.8	Ni 1.8	Cu 1.8	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr –
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	Xe –
Cs 0.7	Ba 0.9	57–71 1.1–1.2	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 1.8	Bi 1.9	Po 2.0	At 2.2	Rn –
Fr 0.7	Ra 0.9																

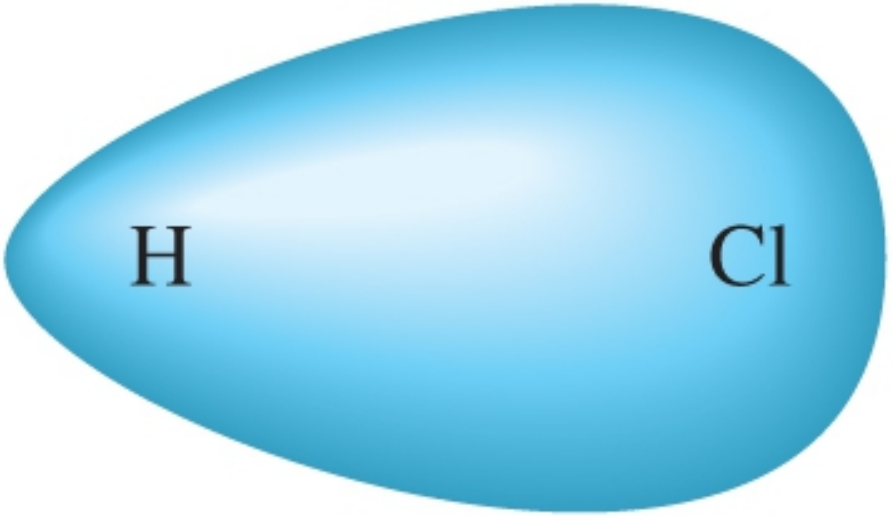
•With a large EN difference (such as between metals and non-metals),
the more electronegative atom takes the electrons from the other atom and forms ions.

•If the ENs are identical, both have the same attraction, and the bonding electrons are shared equally. (non-polar covalent bonds)

•For small EN differences, the electrons are shared, but not equally (polar covalent bonds)



(a)



(b)

Polar (covalent) bonds have a slight positive charge on one end, and a slight negative charge on the other end.

The more EN atom pulls the bonding electrons closer to itself, which creates the slight negative charge.

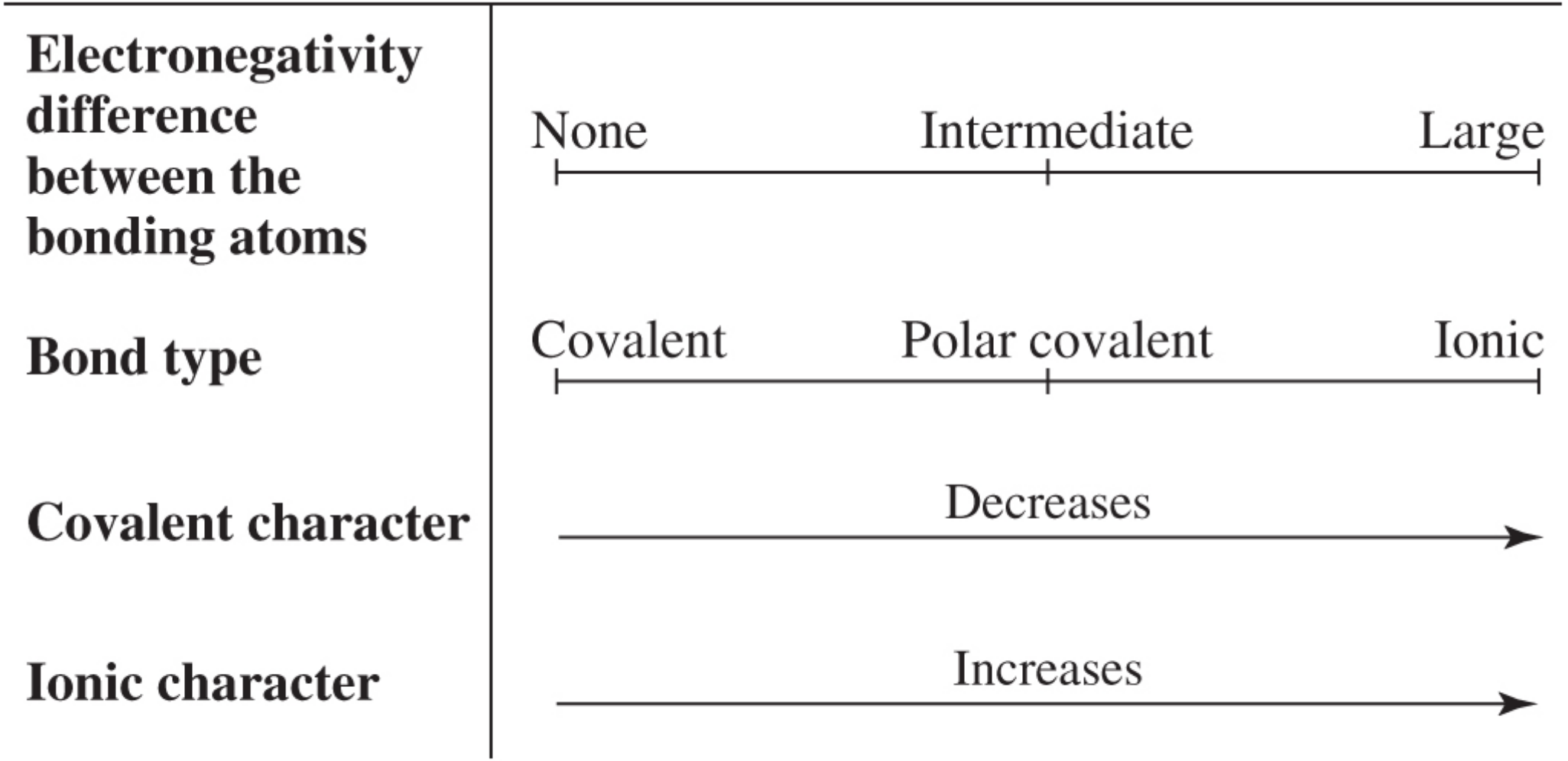
The less EN atom then has a slight positive charge.

This is called a dipole (two poles).

EN difference	***Bond Type***
0 – 0.3	Non-polar (covalent)
0.3 – 1.7	Polar (covalent)
1.7 +	Ionic

Electronegativity values for elements are listed in tables

$M^+ X:^-$	$\overset{\delta+\ \delta-}{Y:X}$	X:X
Ionic (full charges)	Polar covalent (partial charges)	Nonpolar covalent (no charges)
Electron transfer	Unequal sharing of electrons	Equal sharing of electrons

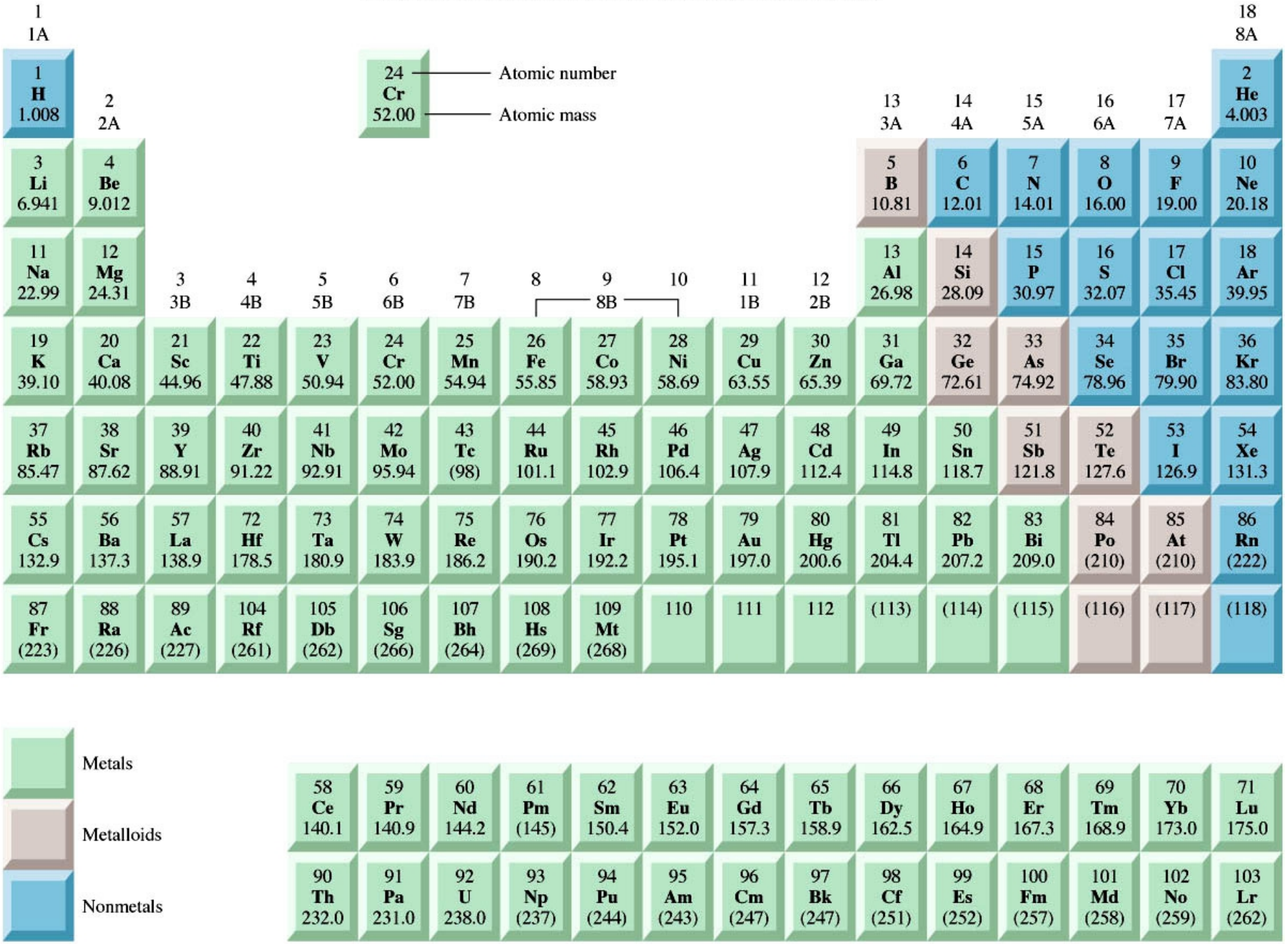


In many cases, the type of bond formed may be predicted based on the periodic table:

- Metal/metal bond – metallic

- Metal/non-metal bond – usually ionic

- Non-metal/non-metal – covalent
  - element bonded to itself – non-polar
  - element bonded to an atom adjacent on the Periodic Table – probably non-polar (covalent)
  - element bonded to an atom two or more spaces apart on PT – probably polar (covalent)



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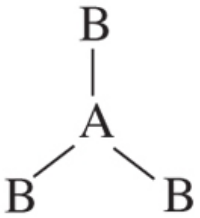
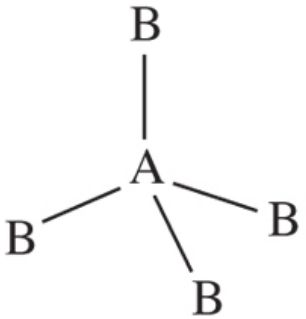
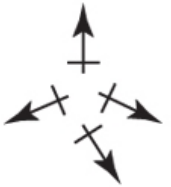
Polar Molecules

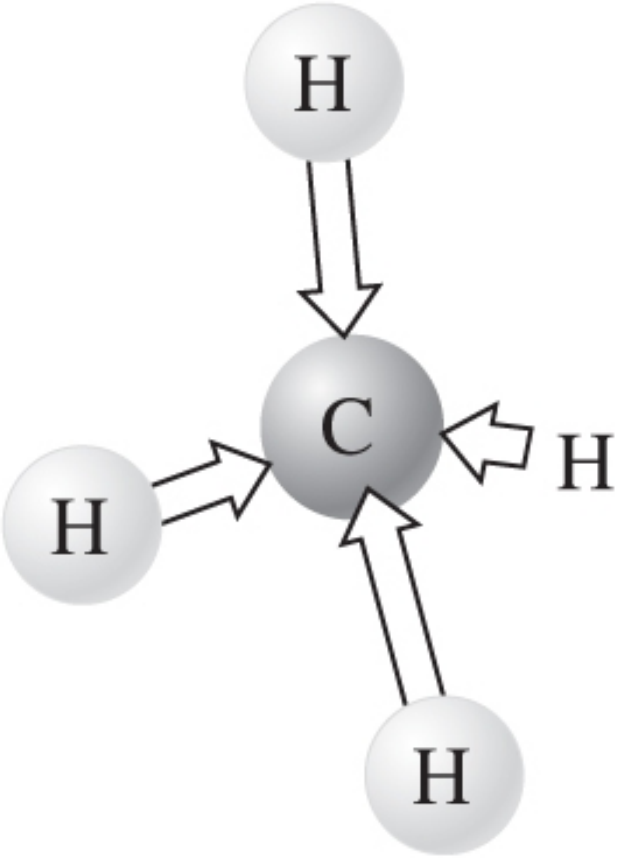
- Molecules that have a dipole moment – a difference in polarity from one end to the other

- Molecules must have polar bonds or asymmetric unpaired electrons.

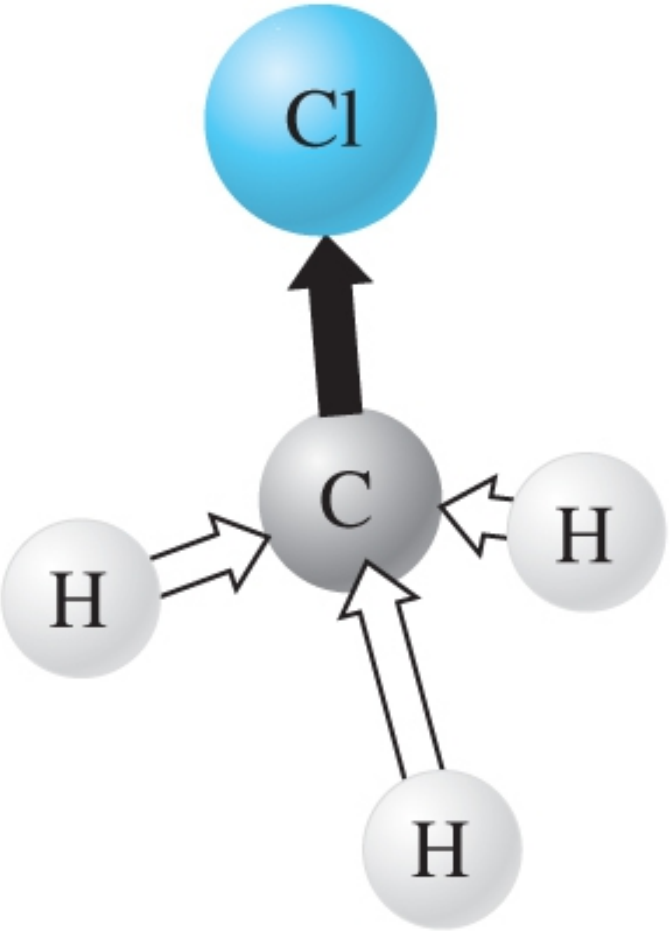
- Molecule must also by asymmetric (not symmetric) to be a polar molecule

- Polar molecules have a attraction to other polar molecules, like a weak ionic bond.

Type		Cancellation of Polar Bonds	Example
Linear molecules with two identical bonds	B—A—B		CO_2
Trigonal planar molecules with three identical bonds			SO_3
Tetrahedral molecules with four identical bonds			CH_4



(a) CH_4, a nonpolar molecule



(b) CH_3Cl, a polar molecule