Chemical Threats
Advanced Chemistry Course

SAND2010-3895P

Chemical Concepts, Part 1

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

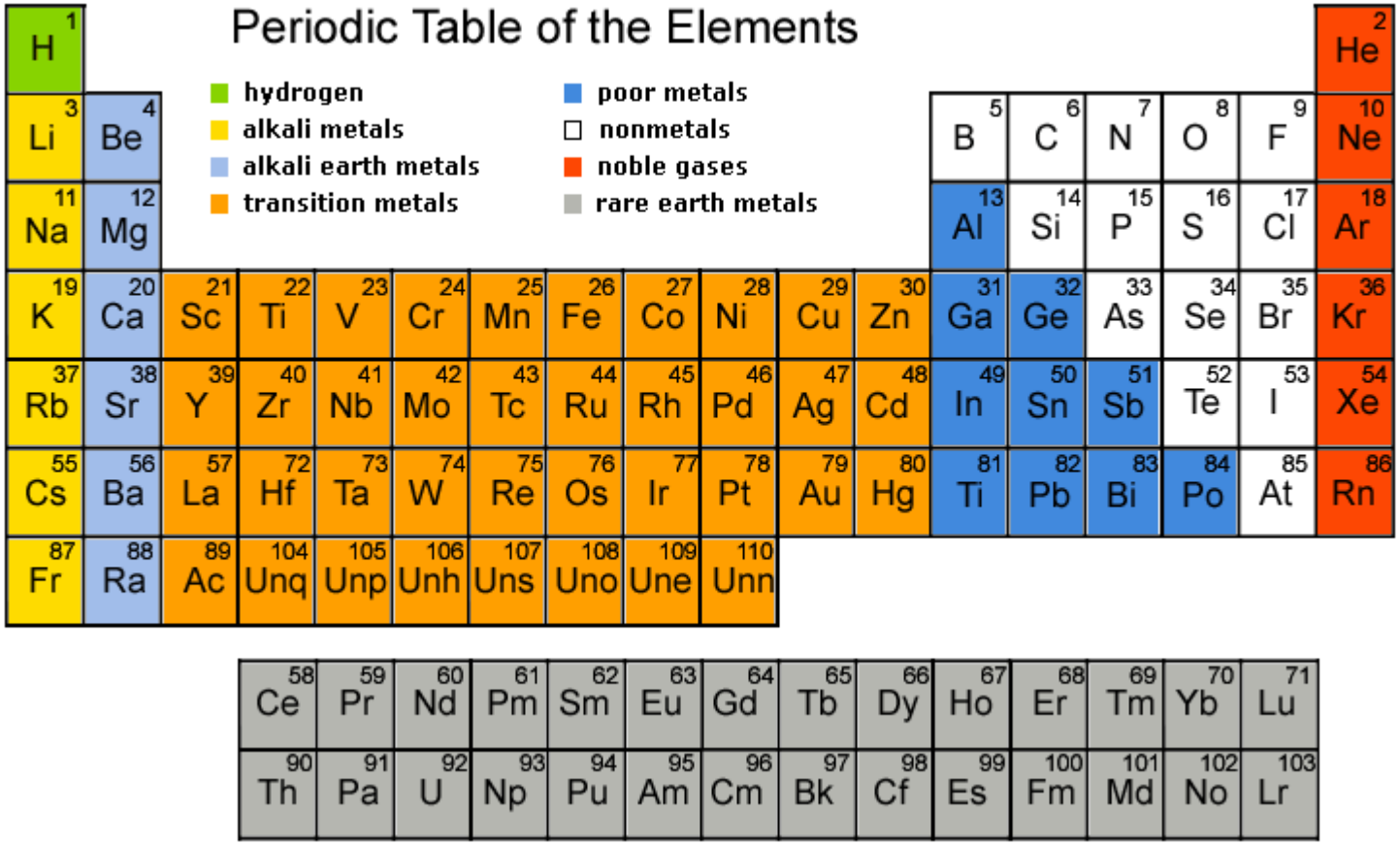
BIOSECURITY ENGAGEMENT PROGRAM

International BIOLOGICAL THREAT REDUCTION

Introduction to Chemistry

- **Periodic Table**
  - Fundamental organization
  - Elements and symbols
  - Protons, Neutrons, Electrons
  - Oxidation States
- **Concepts**
  - Atoms
  - Molecules
  - Balancing Equations

Periodic Table



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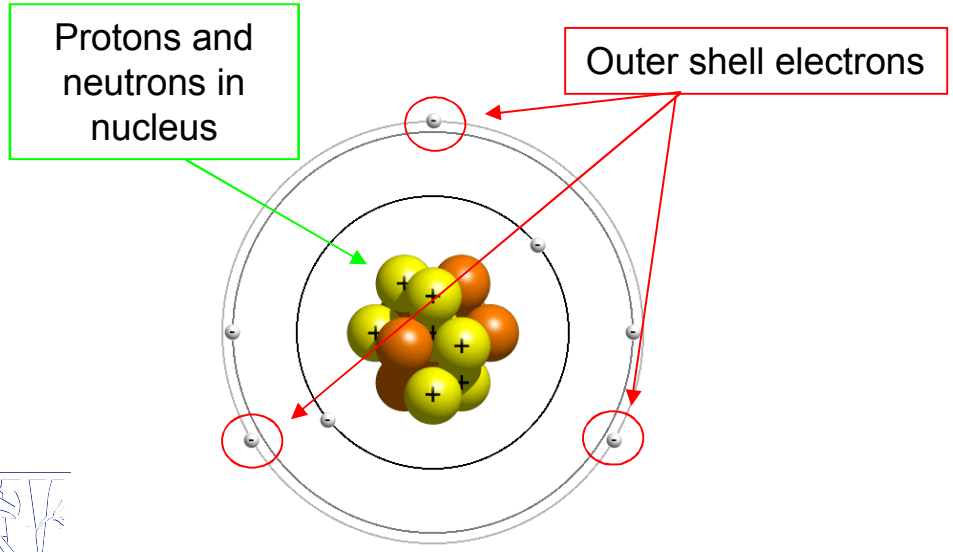
Periodic Table

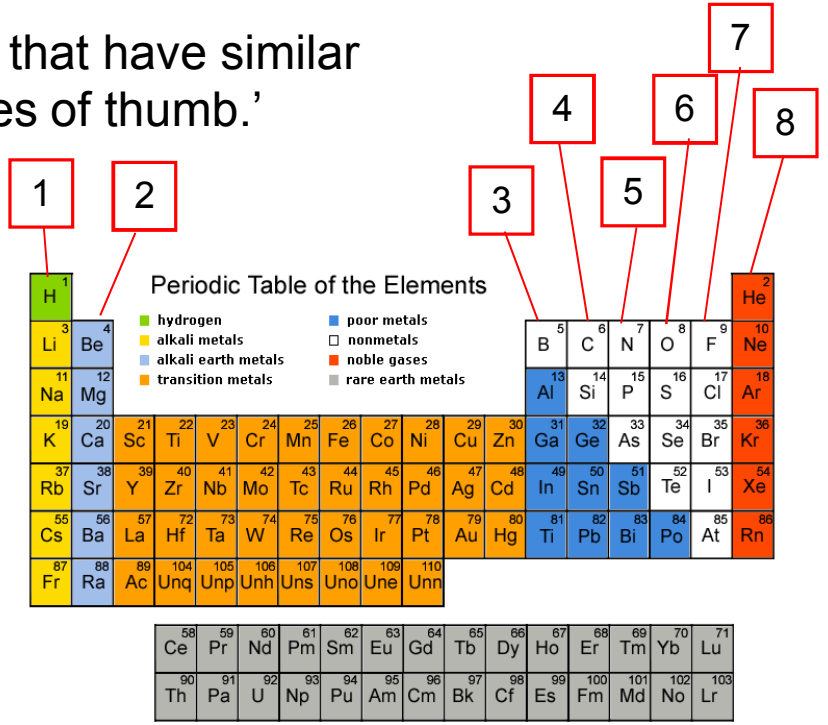
Logical Organization of Elements

1. Elements in a column have similar (but not the same) properties.
2. There are distinct ‘families’ of elements that have similar properties.
3. Properties of elements progress in a predictable manner as one progresses from left to right on the table.
4. Each element has a unique ‘symbol’ which is universal.
5. Each element has a unique atomic number.

Periodic Table

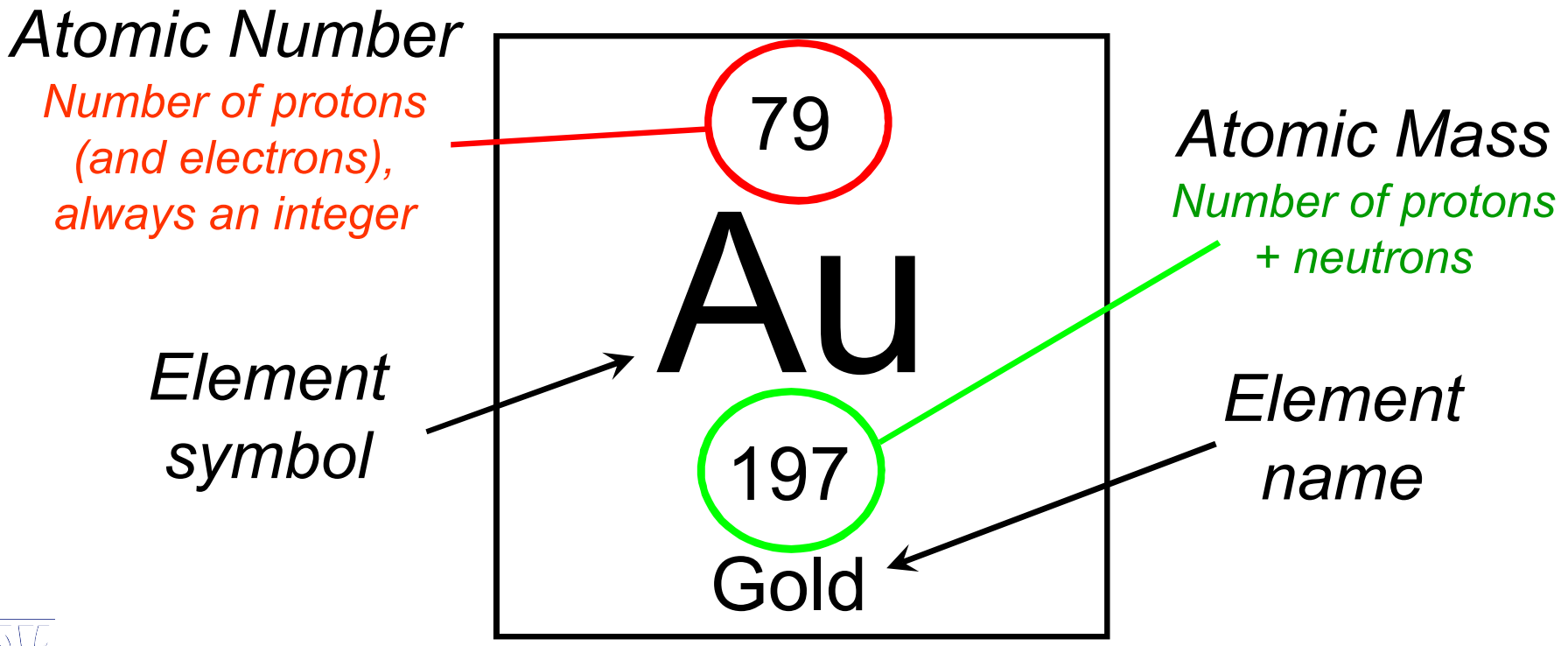
- Elements in a column have similar (but not the same) properties – due to number of electrons in outer orbits.
- There are distinct 'families' of elements that have similar properties – gives rise to 'chemistry rules of thumb.'



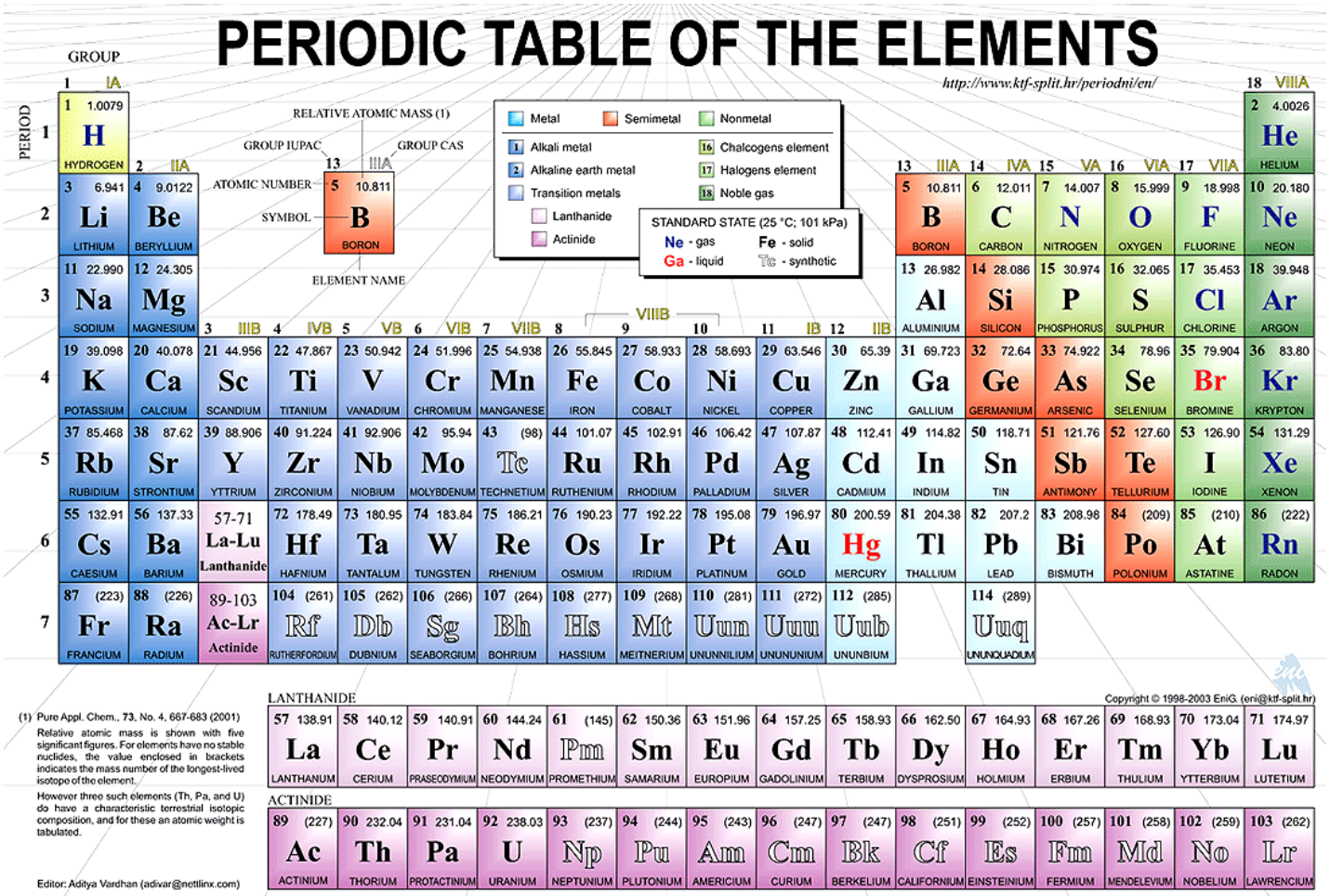


Atomic Symbol

What information can be obtained found from the Atomic Symbol?



Periodic Table



Element Exercise

What day of the month were you born? _____

Using this date as an Atomic Number,

What is the corresponding element? _____

What is the elemental symbol? _____

What is the number of protons in your birth element? _____

What is the number of neutrons in your birth element? _____

How is you birth element found in nature? _____

What is it used for? _____

For more chemistry fun, try the last two digits of your birth year!

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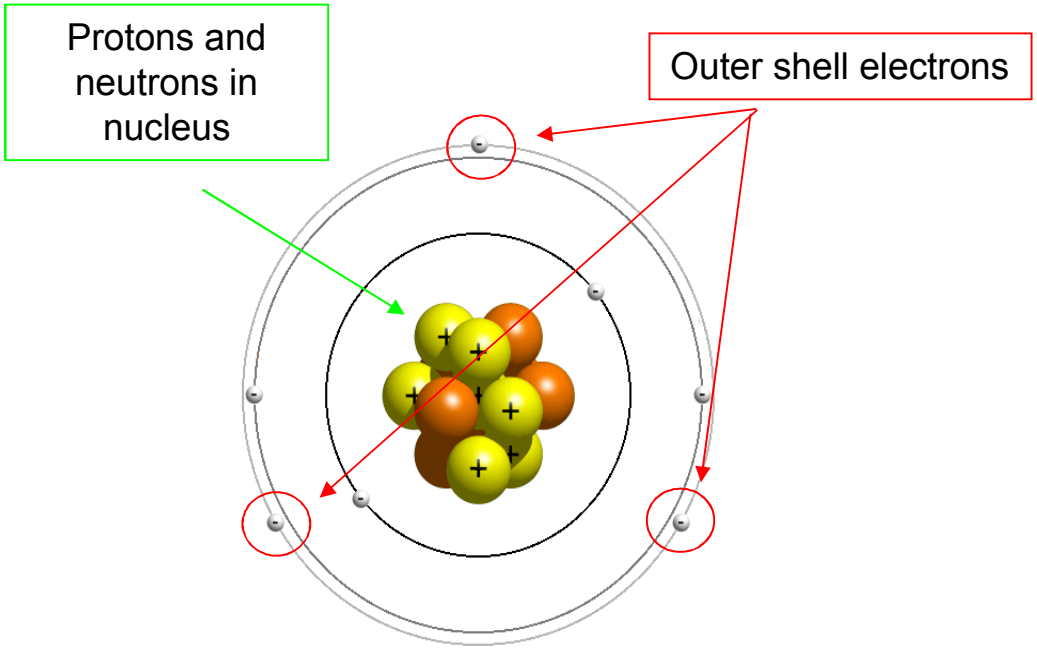
Atomic Model

Nucleus

1. Center of atom, contains most of the atomic mass.
2. Composed of protons, +1 charge, and
3. Neutrons, 0 charge

Orbiting Electrons, -1 charge



For most atoms, the energy minimum is to have 8 electrons in the atomic outer shell.

Atoms will gain or lose electrons to meet this 8 electron goal.

Also, pairs of electrons are energetically more favorable.

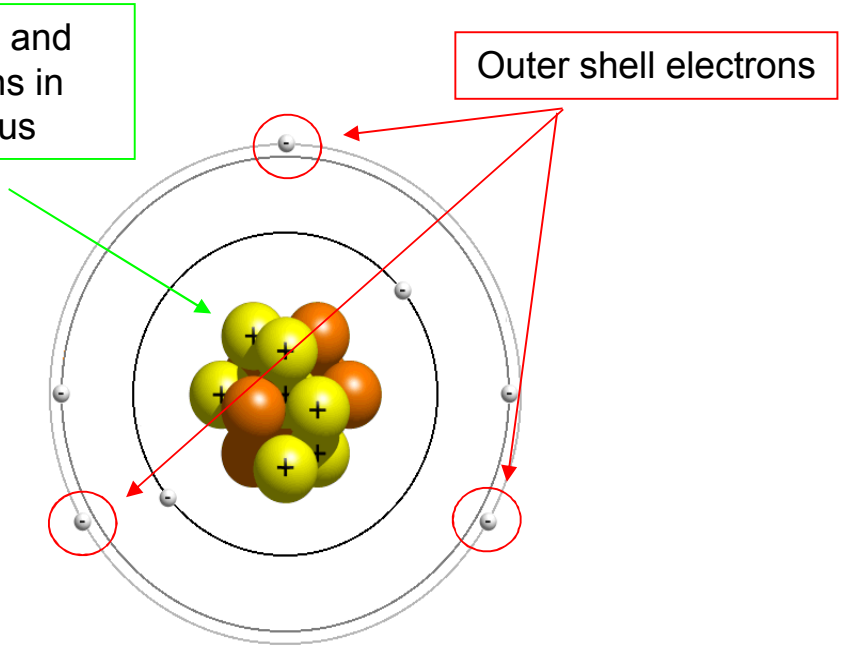
Atomic Model, Explained

Nucleus

1. Number of Protons give each element it's unique character.
2. Number of Neutrons determine nuclear stability.

Orbiting Electrons

1. Form the bonds between atoms.
2. Are the 'reactive part' of the element.

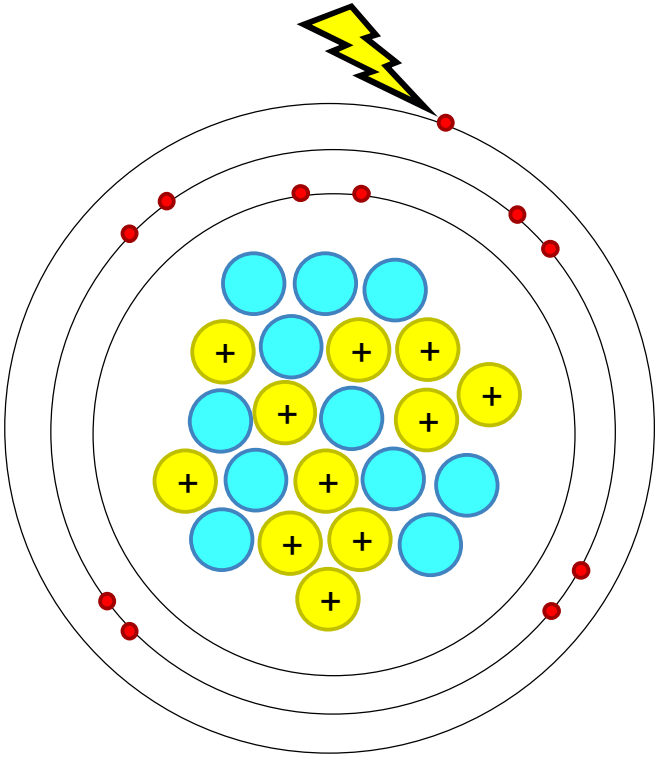


8 Electron Goal; Ionization or Bonding

Ionization: the gain or loss of one or more electrons to satisfy the 8 electron goal.

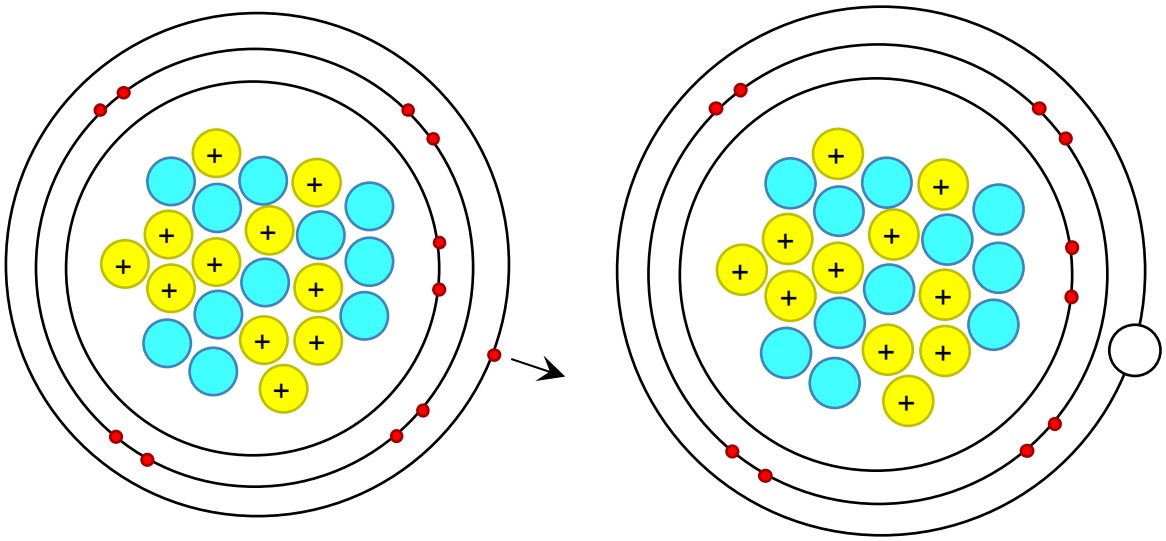
Sodium atom

- 11 protons
- 11 neutrons
- 11 electrons
- 1 electron in the outer shell; not energetically favored.



8 Electron Goal; Ionization

Sodium can lose one electron to achieve the 8 electron goal, the 'full outer shell.'

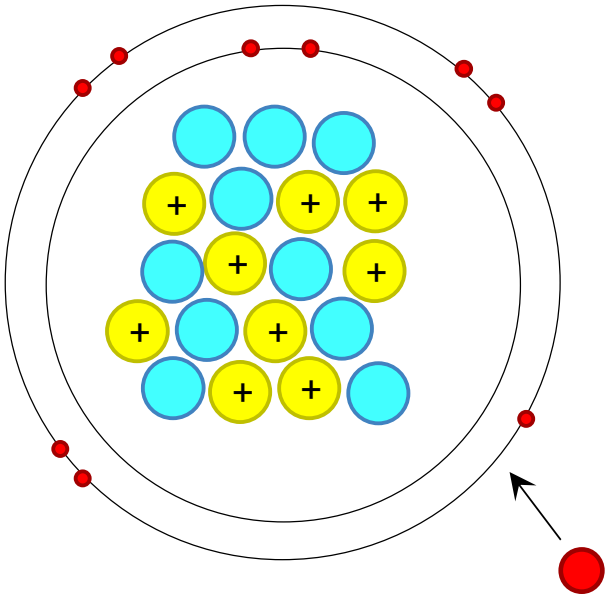


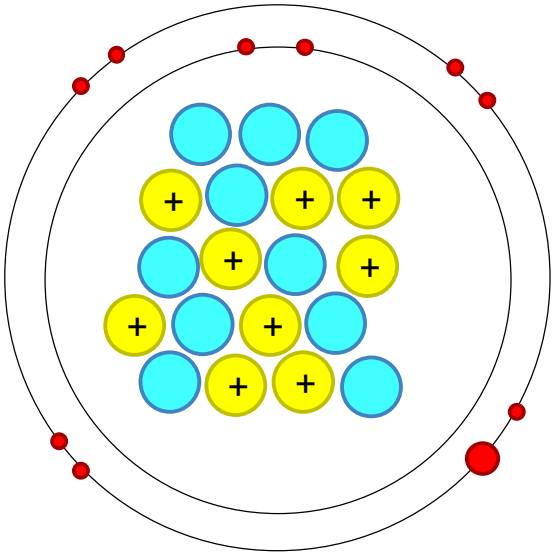
Sodium ion

- 11 protons
- 11 neutrons
- 10 electrons
- Net +1 charge
- Energetically favored.

8 Electron Goal; Ionization

Fluorine can gain one electron to achieve the 8 electron goal, the 'full outer shell.'

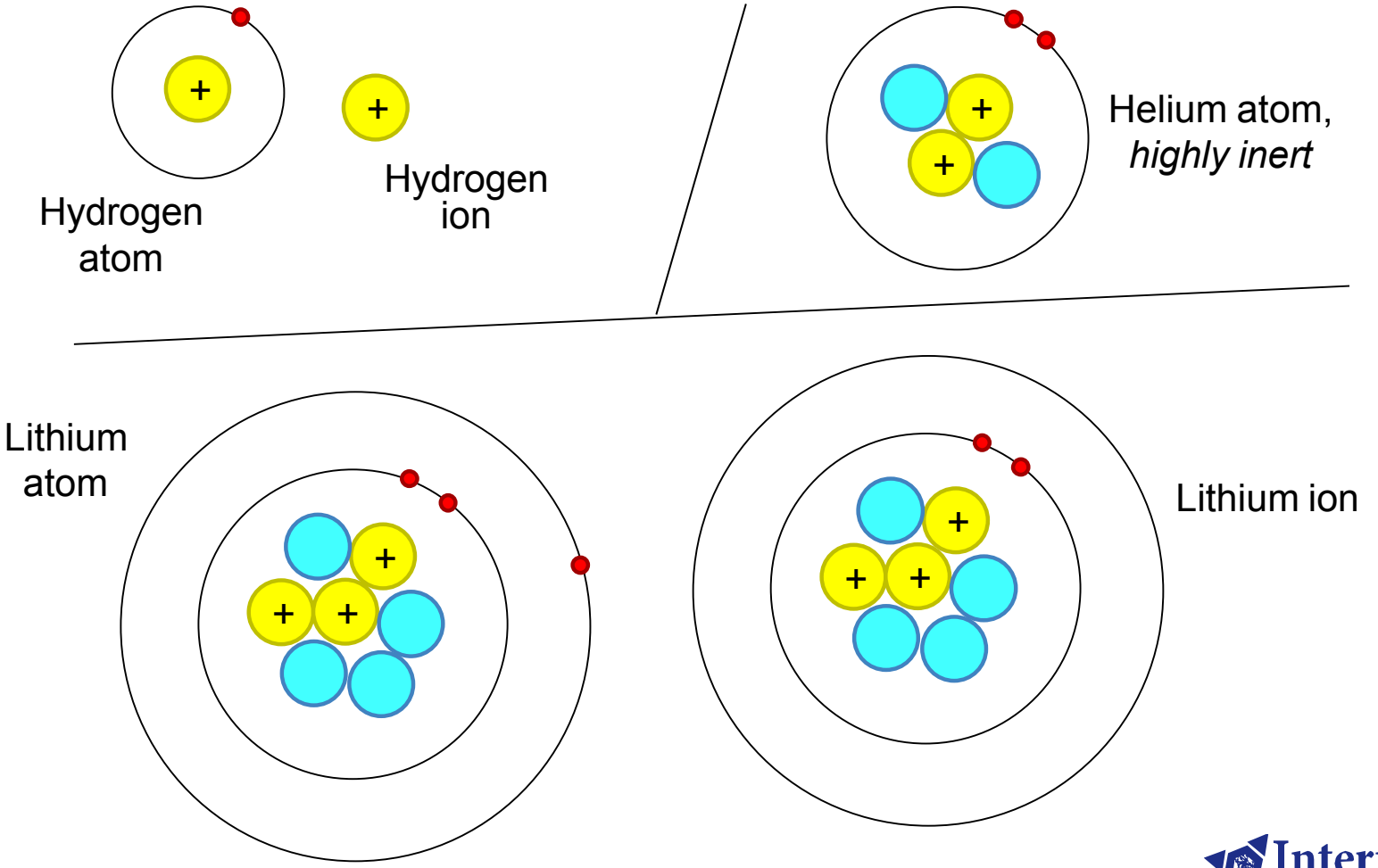




Fluoride ion

- 9 protons
- 10 neutrons
- 10 electrons
- Net -1 charge
- Energetically favored.

0 or 2 Electron Goal Exceptions

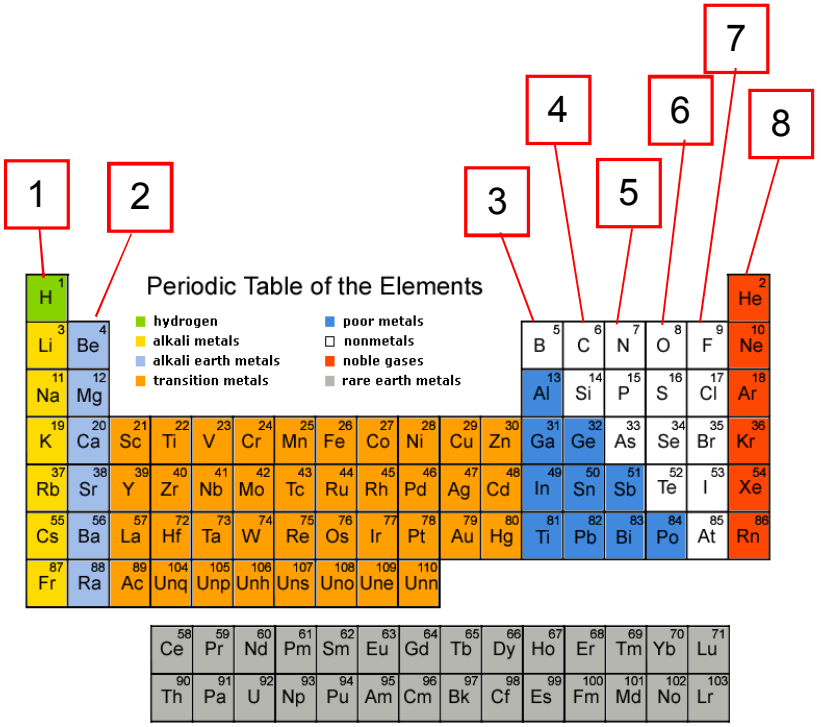


Electrons; Ionization

Elements in columns 1 and 2 readily <u>lose</u> electrons.

Elements in columns 6 and 7 readily <u>gain</u> electrons.

Elements in column 8 have their outer shell 'satisfied', so are <u>unreactive</u> or <u>inert</u>. These are the noble gases.



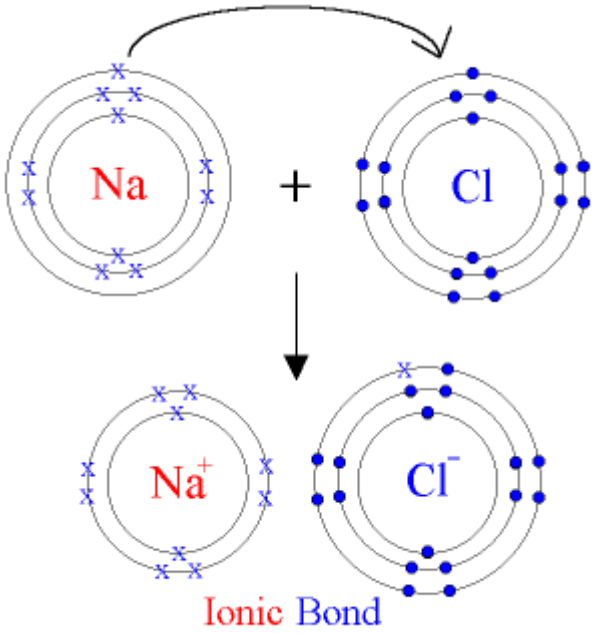
So, more correctly, atoms tend to the noble gas core they are closest to in the periodic table.

Ionic Bonds

Elements widely spaced in periodic table will transfer electrons, resulting in ‘ionic’ bonding.

Sodium atoms would readily give up an electron to a chlorine atom, resulting in the ionic compound sodium chloride.

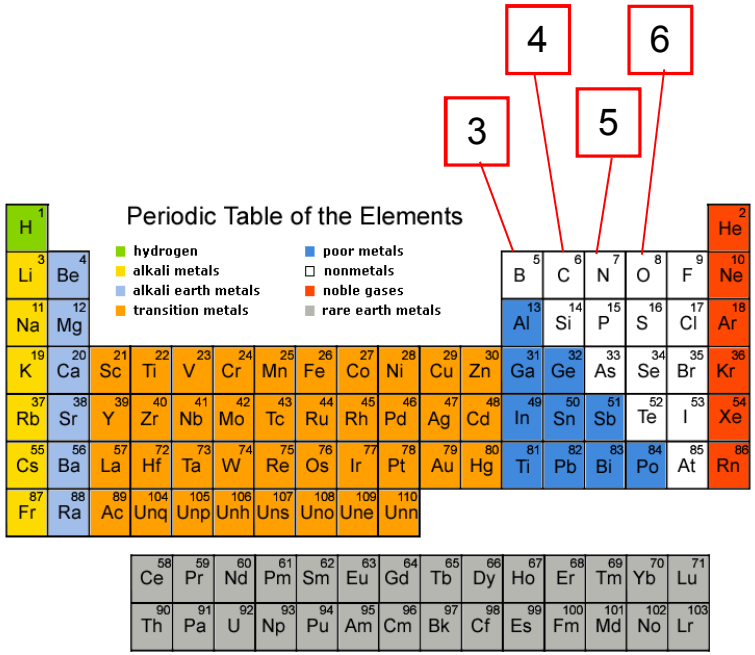
Ionic materials are held together by electrostatics.



Covalent Bonding

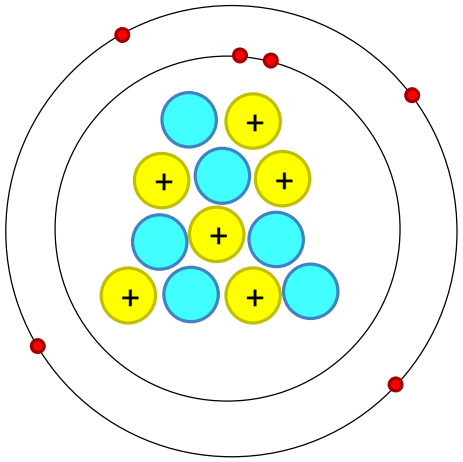
What about Columns 3, 4, 5 and to some extent, 6?

Giving up or gaining a lot of electrons is not energetically favorable.



Carbon atom

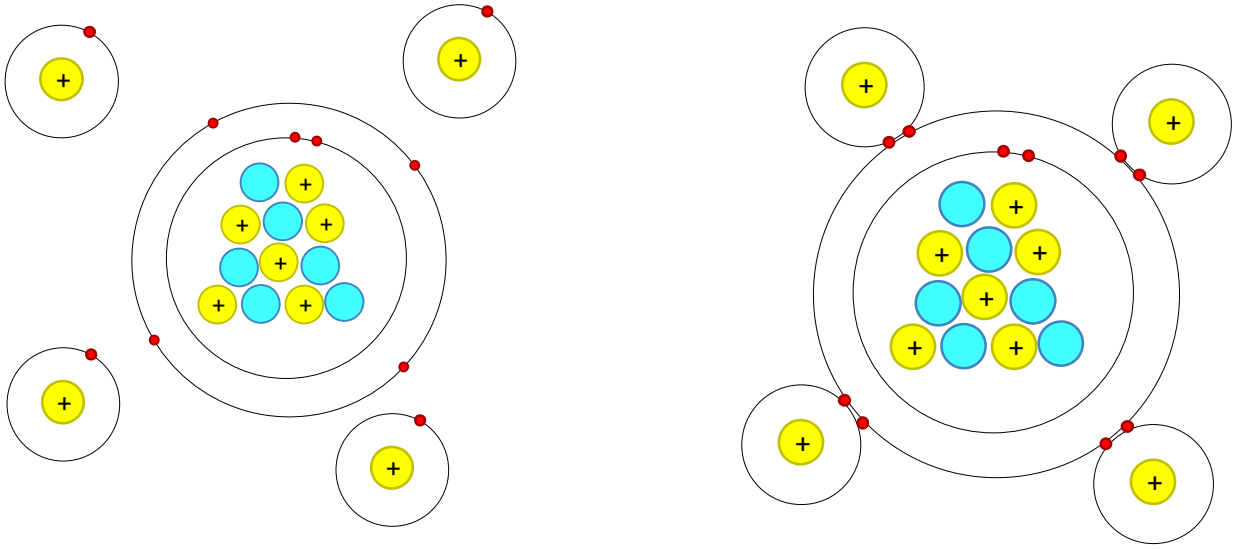
- 6 protons
- 6 neutrons
- 6 electrons
- 4 unpaired electrons



Electron Sharing, or Covalent Bonding

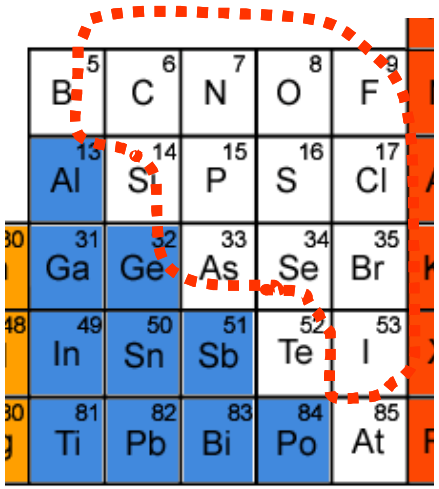
Electrons may be shared by atoms; the electron pairs are considered to satisfy the electronic requirements of both atoms.

Four Hydrogen atoms can bond to one carbon atom:



Covalent Bonding

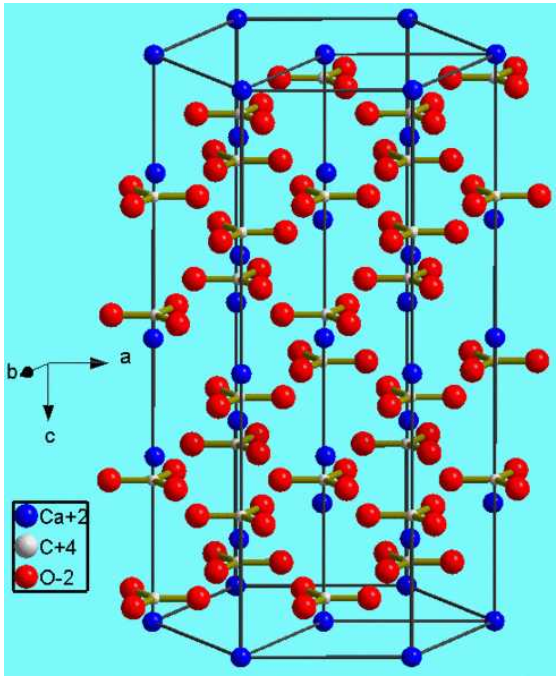
1. Covalent, or shared electron bonding, occurs in main group elements that are close in the periodic table.
2. Covalent bonds are stronger than ionic bonds.
3. Some atoms form multiple covalent bonds (double or triple bonds).
4. *Covalent bonds form the basis of organic chemistry*

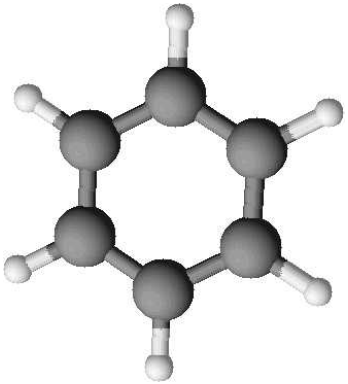


Compounds

Chemical Compounds are composed of two or more chemical elements.

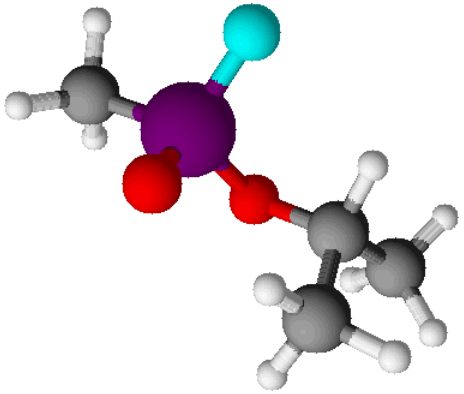
$CaCO_3$, Calcium carbonate





C_6H_6, Benzene

$PO_2FC_4H_{10}$, Sarin

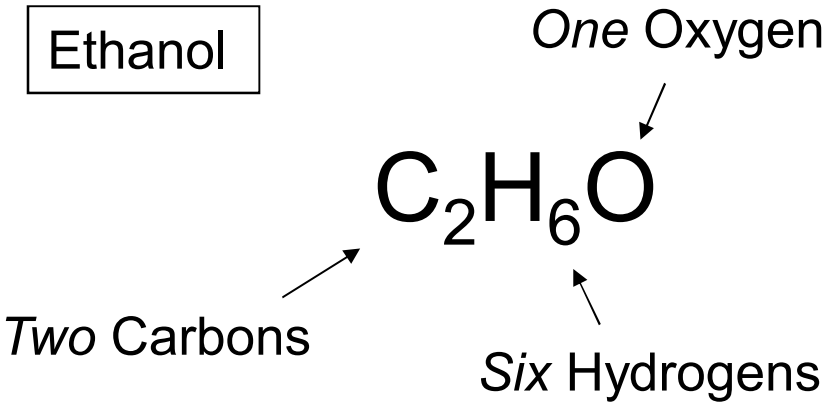


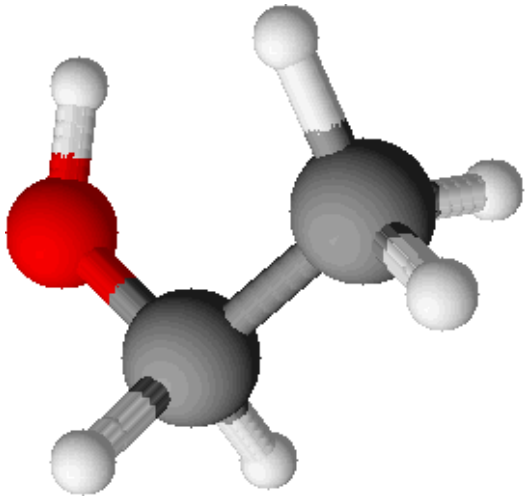
Chemical Formulas

Chemical Formulas are shorthand notation of composition.

- Subscripts denote number of atoms.

Ethanol





Chemical Formulas

Chemical Formulas are shorthand notation of composition.

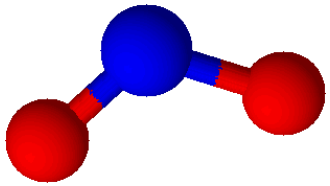
Nitrite

Net negative charge

NO_2^-

One Nitrogen

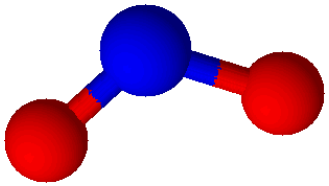
Two Oxygens

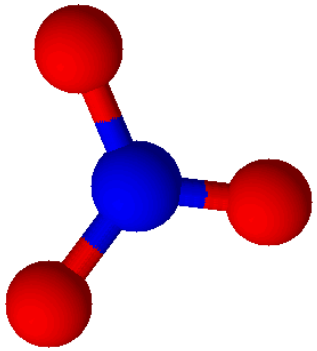


Oxidation States

- Some atoms can have differing number of covalent bonds depending on what it is bonded to.
- This number of bonds is the ‘oxidation state’ of the atom.
- Some oxidation states are more reactive than others.

Compound	Formula	Oxidation state of Nitrogen
Nitrite	NO_2^-	+3
Nitrate	NO_3^-	+5

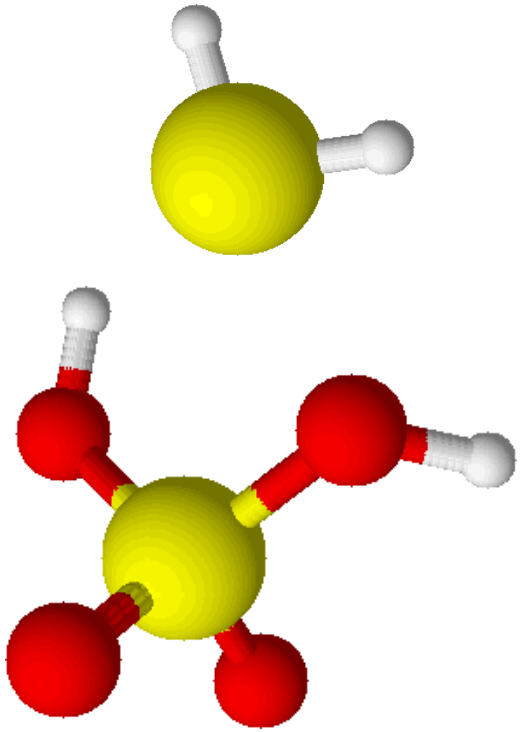




Oxidation States

- Some atoms have a large number of possible oxidation states.

Compound	Formula	Oxidation state of Sulfur
Hydrogen sulfide	H_2S	-2
Sulfuric acid	H_2SO_4	+6



Oxidation States

From the formula, we can determine the oxidation state of the atoms.

Method to Determine Oxidation State of nitrogen in nitrite.

NO_2^-

- Any net charge on the compound? _____
- Number of oxygen atoms: ____
  - **Oxygen is worth -2, so net charge contributed by oxygen atoms ____ ((# of oxygens present) x -2) = _____**
- If overall charge in nitrite is ____, then the charge on the nitrogen must be:

Charge on the nitrogen = net charge – (# of oxygens x -2)

Charge on the nitrogen = (-1 – (2 x -2))

= (-1 – (-4))

= +3

Oxidation States

Method to Determine Oxidation State of chlorine in perchlorate.

ClO_4^-

- Any net charge on the compound? _____
- Number of oxygen atoms: ____
  - **Oxygen is worth -2, so net charge contributed by oxygen atoms ____ ((# of oxygens present) x -2) = _____**

- If overall charge on perchlorate is ____, then the charge on the chlorine must be:

  Charge on the chlorine = net charge – (# of oxygens x -2)

  Charge on the chlorine = (-1 – (4 x -2))

  = (-1 – (-8))

  = +7

Flexible Oxidation States

Many main group atoms exhibit several oxidations states:

Element	Some Oxidation States observed
Nitrogen	+3, +5, -3
Oxygen	-1, -2
Phosphorus	+3, +5
Sulfur	+4, +6, -2
Chlorine	+1, +3, +5, +7, -1

Example

Pool chemical/muriatic acid reaction to generate chlorine gas.

$$OCl^- + Cl^- \longrightarrow Cl_2$$

	Hypochlorite	Chloride	Chlorine
Oxidation State	+1	-1	0

Summary

Chemistry is a Logical Science

- **Element's position in the periodic table can tell you immediately:**
  - Expected properties
  - Likely Oxidation State and number of states readily accessible
  - Whether it forms ionic or covalent bonds.
  - How many electrons are present in an elements outer shell.