



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.



Introduction to Chemistry

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

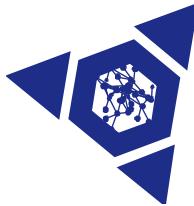




Periodic Table

Periodic Table of the Elements

⁵⁸ Ce	⁵⁹ Pr	⁶⁰ Nd	⁶¹ Pm	⁶² Sm	⁶³ Eu	⁶⁴ Gd	⁶⁵ Tb	⁶⁶ Dy	⁶⁷ Ho	⁶⁸ Er	⁶⁹ Tm	⁷⁰ Yb	⁷¹ Lu
⁹⁰ Th	⁹¹ Pa	⁹² U	⁹³ Np	⁹⁴ Pu	⁹⁵ Am	⁹⁶ Cm	⁹⁷ Bk	⁹⁸ Cf	⁹⁹ Es	¹⁰⁰ Fm	¹⁰¹ Md	¹⁰² No	¹⁰³ Lr



Periodic Table

Logical Organization of Elements

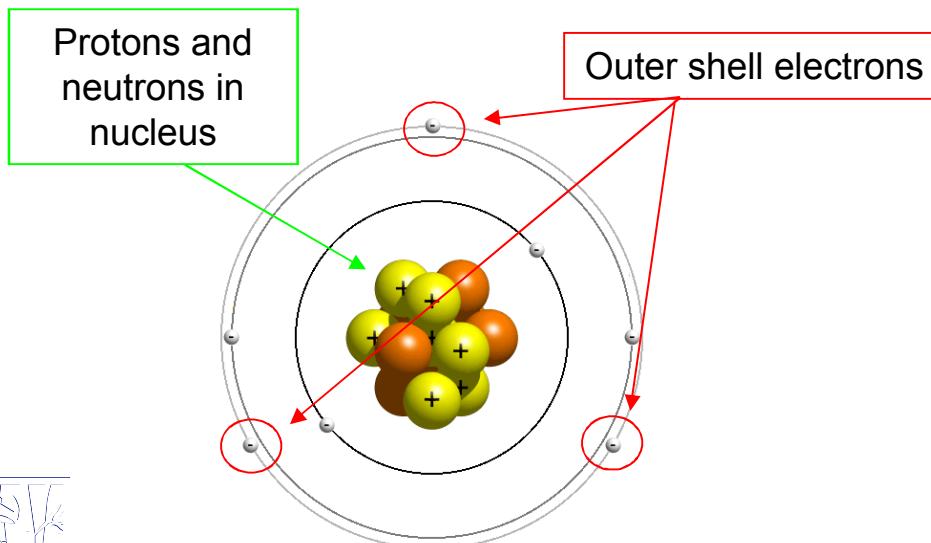
1. Elements in a column have similar (but not the same) properties.
2. There are distinct 'families' of elements that have similar properties.
3. Properties of elements progress in a predictable manner as one progresses from left to right on the table.
4. Each element has a unique 'symbol' which is universal.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



that have similar
es of thumb.'

1 2

3 4 5 6 7 8

Periodic Table of the Elements

■ hydrogen ■ poor metals
 ■ alkali metals ■ nonmetals
 ■ alkali earth metals ■ noble gases
 ■ transition metals ■ rare earth metals

H	Li	Be	Na	Mg	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr							
3	4	11	12	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36								
Li	Be	Na	Mg	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr								
Rb	Sr	Y	Zr	Nb	Mo	Tc	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55								
Cs	Ba	La	Hf	Ta	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88									
Fr	Ra	Ac	Unq	104	105	106	107	108	109	110	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr					
58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		



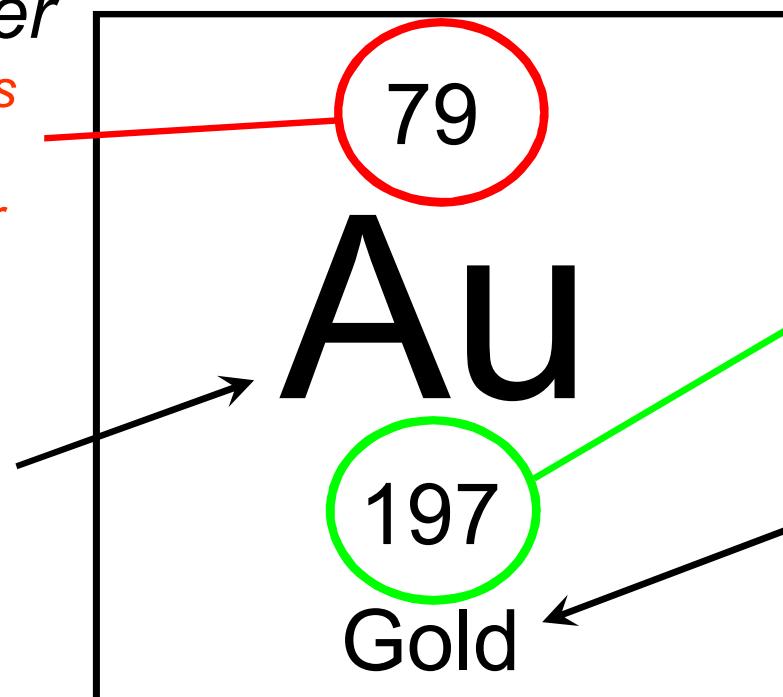
Atomic Symbol

What information can be obtained found from the Atomic Symbol?

Atomic Number

*Number of protons
(and electrons),
always an integer*

*Element
symbol*



Atomic Mass

*Number of protons
+ neutrons*

*Element
name*



Periodic Table

PERIODIC TABLE OF THE ELEMENTS

<http://www.ktf-split.hr/periodni/en/>

PERIOD	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
GROUP	IA	IIA	IIIA	IVB	VB	VIIB	VIIIB	VIIIB	VIIIB	IB	IB	IB	IIIA	IVA	VA	VIA	VIIA	VIIIA
1	1 1.0079 H HYDROGEN	2 6.941 Li LITHIUM	3 9.0122 Be BERYLLIUM	4 10.811 B BORON	5 10.811 B BORON	6 12.011 C CARBON	7 14.007 N NITROGEN	8 15.999 O OXYGEN	9 18.998 F FLUORINE	10 20.180 Ne NEON	11 22.990 Na SODIUM	12 24.305 Mg MAGNESIUM	13 10.811 B BORON	14 12.011 C CARBON	15 14.007 N NITROGEN	16 15.999 O OXYGEN	17 18.998 F FLUORINE	18 20.180 Ne NEON
2	19 39.098 K POTASSIUM	20 40.078 Ca CALCIUM	21 44.956 Sc SCANDIUM	22 47.867 Ti TITANIUM	23 50.942 V VANADIUM	24 51.996 Cr CHROMIUM	25 54.938 Mn MANGANESE	26 55.845 Fe IRON	27 58.933 Co COBALT	28 58.693 Ni NICKEL	29 63.546 Cu COPPER	30 65.39 Zn ZINC	31 69.723 Al ALUMINIUM	32 72.64 Si SILICON	33 74.922 P PHOSPHORUS	34 78.96 S SULPHUR	35 79.904 Cl CHLORINE	36 83.80 Ar ARGON
3	37 85.468 Rb RUBIDIUM	38 87.62 Sr STRONTIUM	39 88.906 Y YTTRIUM	40 91.224 Zr ZIRCONIUM	41 92.906 Nb NIOBUM	42 95.94 Mo MOLYBDENUM	43 (98) Tc TECHNETIUM	44 101.07 Ru RUTHENIUM	45 102.91 Rh RHIDIUM	46 106.42 Pd PALLADIUM	47 107.87 Ag SILVER	48 112.41 Cd CADMIUM	49 114.82 In INDIUM	50 118.71 Sn TIN	51 121.76 Sb ANTIMONY	52 127.60 Te TELLURIUM	53 126.90 I IODINE	54 131.29 Xe XENON
4	55 132.91 Cs CAESIUM	56 137.33 Ba BARIUM	57-71 La-Lu Lanthanide	72 178.49 Hf HAFNIUM	73 180.95 Ta TANTALUM	74 183.84 W TUNGSTEN	75 186.21 Re RHENIUM	76 190.23 Os OSMIUM	77 192.22 Ir IRIDIUM	78 195.08 Pt PLATINUM	79 196.97 Au GOLD	80 200.59 Hg MERCURY	81 204.38 Tl THALLIUM	82 207.2 Pb LEAD	83 208.98 Bi BISMUTH	84 (209) Po POLONIUM	85 (210) At ASTATINE	86 (222) Rn RADON
5	87 (223) Fr FRANCIUM	88 (226) Ra RADIUM	89-103 Ac-Lr Actinide	104 (261) Rf RUTHERFORDIUM	105 (262) Db DUBNIUM	106 (266) Sg SEABORGIUM	107 (264) Bh BOHRIUM	108 (277) Hs MEITNERIUM	109 (268) Mt UNUNIUM	110 (281) Uum UNUNIUM	111 (272) Uuu UNUNIUM	112 (285) Uub UNUNIUM	114 (289) Uuq UNUNQUIDIUM					
6																		
7																		

(1) Pure Appl. Chem., 73, No. 4, 667-683 (2001)

Relative atomic mass is shown with five significant figures. For elements have no stable nuclides, the value enclosed in brackets indicates the mass number of the longest-lived isotope of the element.

However three such elements (Th, Pa, and U) do have a characteristic terrestrial isotopic composition, and for these an atomic weight is tabulated.

Editor: Aditya Vardhan (adivar@netlinx.com)

LANTHANIDE

57 138.91 La LANTHANUM	58 140.12 Ce CERIUM	59 140.91 Pr PRASEODYMIUM	60 144.24 Nd NEODYMIUM	61 (145) Pm PROMETHIUM	62 150.36 Sm SAMARIUM	63 151.96 Eu EUROPIUM	64 157.25 Gd GADOLINIUM	65 158.93 Tb TERBIUM	66 162.50 Dy DYSPROSIUM	67 164.93 Ho HOLMIUM	68 167.26 Er ERBIUM	69 168.93 Tm THULIUM	70 173.04 Yb YTTERBIUM	71 174.97 Lu LUTETIUM
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ACTINIDE

89 (227) Ac ACTINIUM	90 232.04 Th THORIUM	91 231.04 Pa PROTACTINIUM	92 238.03 U URANIUM	93 (237) Np NEPTUNIUM	94 (244) Pu PLUTONIUM	95 (243) Am AMERICIUM	96 (247) Cm CURIUM	97 (247) Bk BERKELIUM	98 (251) Cf CALIFORNIUM	99 (252) Es EINSTEINIUM	100 (257) Fm FERMIUM	101 (258) Md MENDELEVIUM	102 (259) No NOBELIUM	103 (262) Lr LAWRENCEUM
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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 your birth element found in nature? _____

What is it used for? _____

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

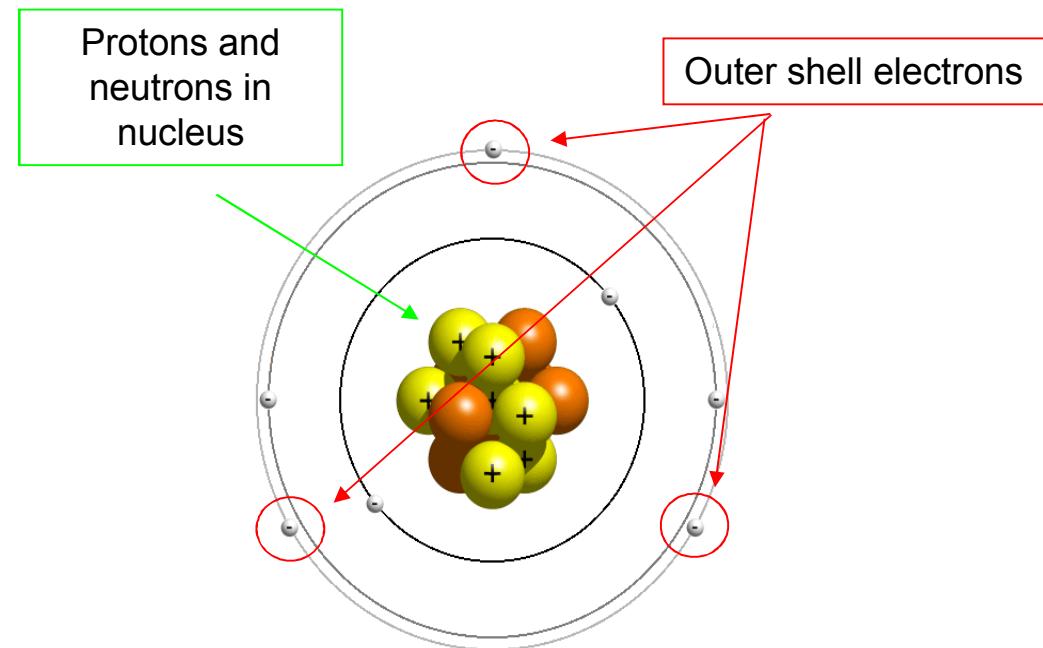


Atomic Model

Nucleus

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

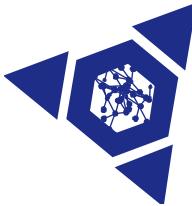
Orbiting Electrons, -1 charge



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.



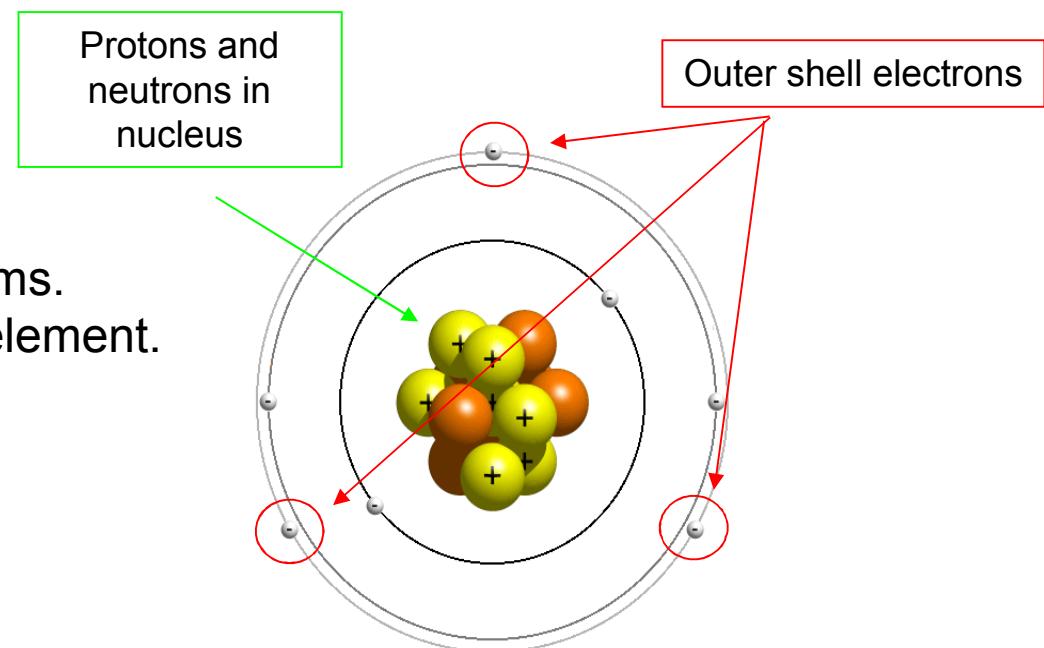
Atomic Model, Explained

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.



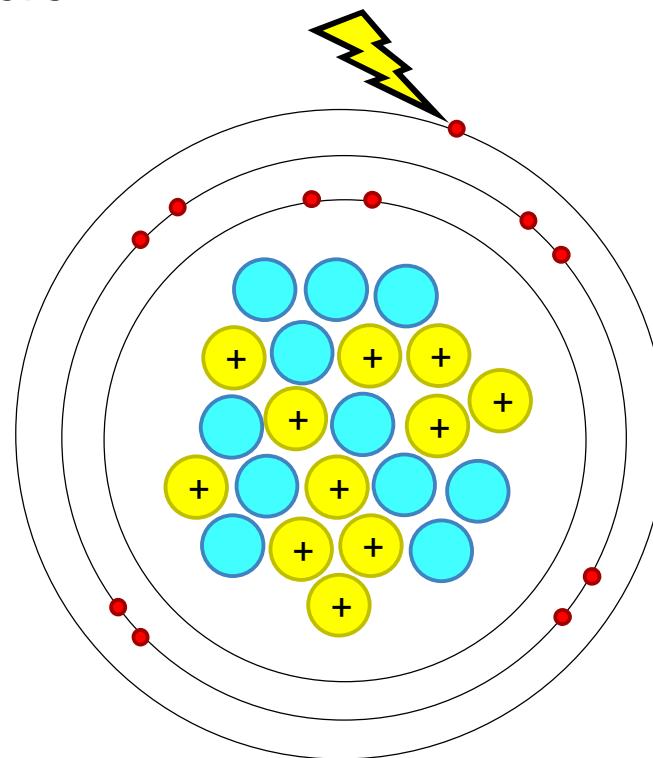


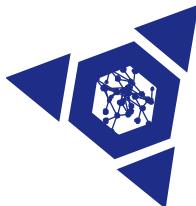
8 Electron Goal; Ionization or Bonding

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

Sodium atom

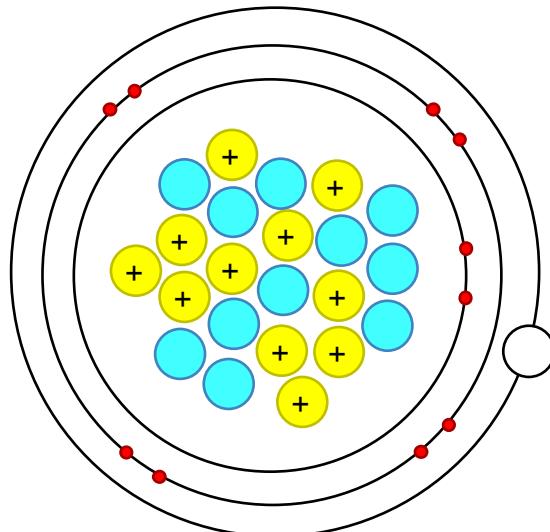
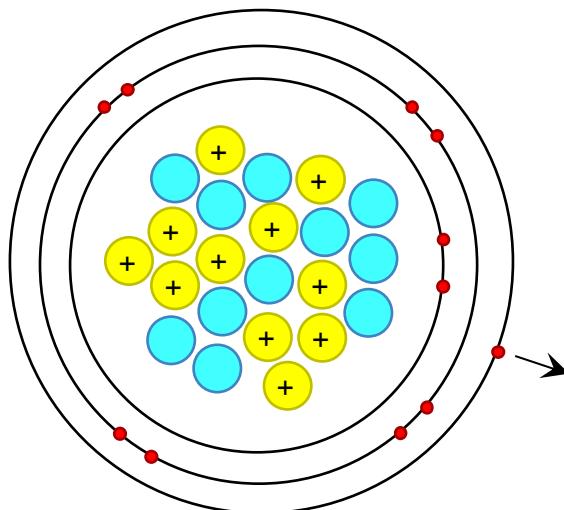
- 11 protons 
- 11 neutrons 
- 11 electrons 
- 1 electron in the outer shell;
not energetically favored.





8 Electron Goal; Ionization

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



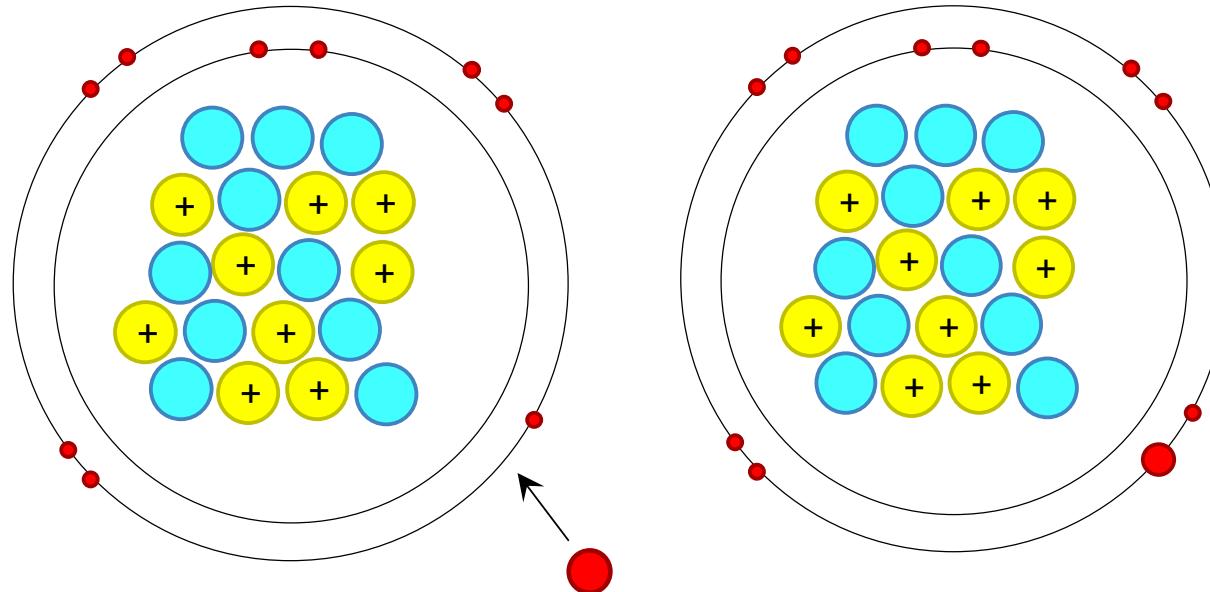
Sodium ion

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



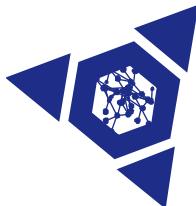
8 Electron Goal; Ionization

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

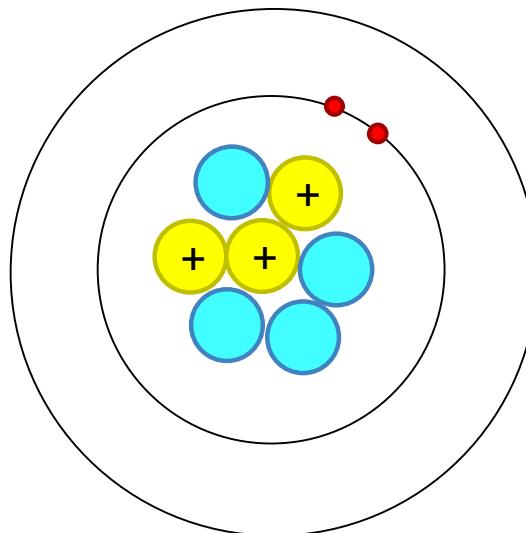
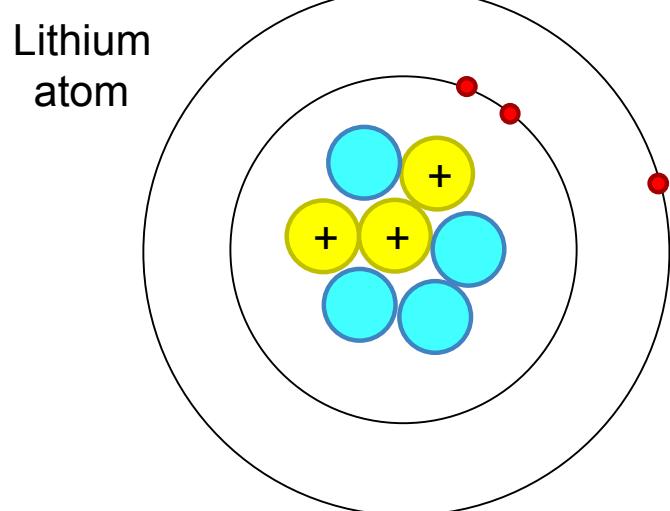
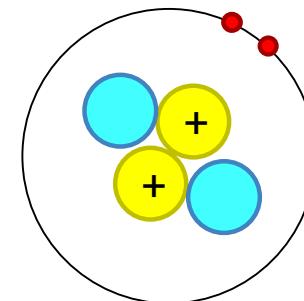
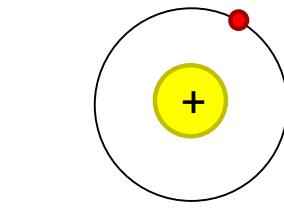


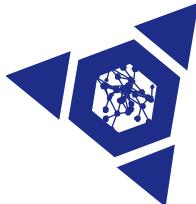
Fluoride ion

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



0 or 2 Electron Goal Exceptions



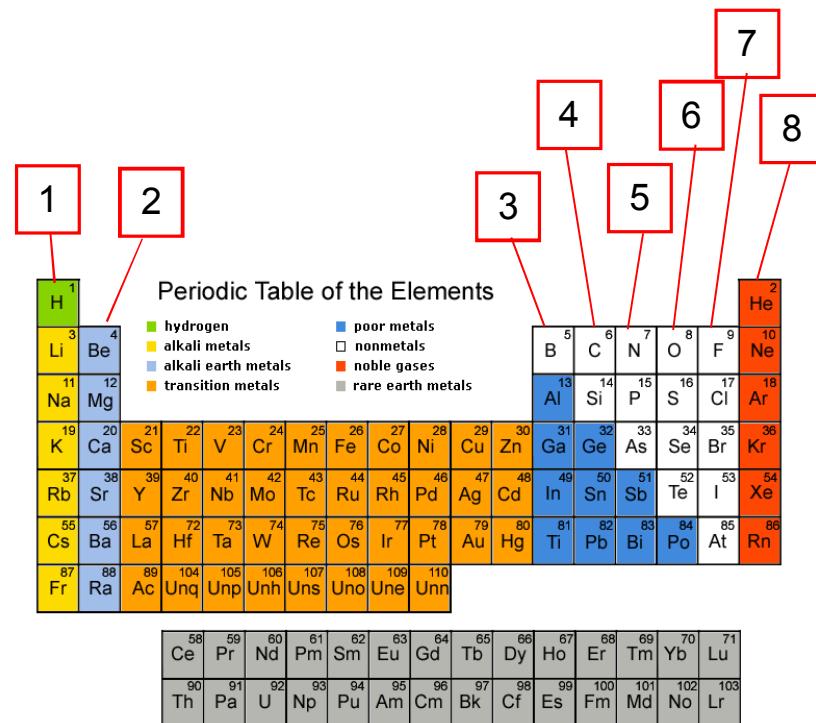


Electrons; Ionization

Elements in columns 1 and 2 readily lose electrons.

Elements in columns 6 and 7 readily gain electrons.

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



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

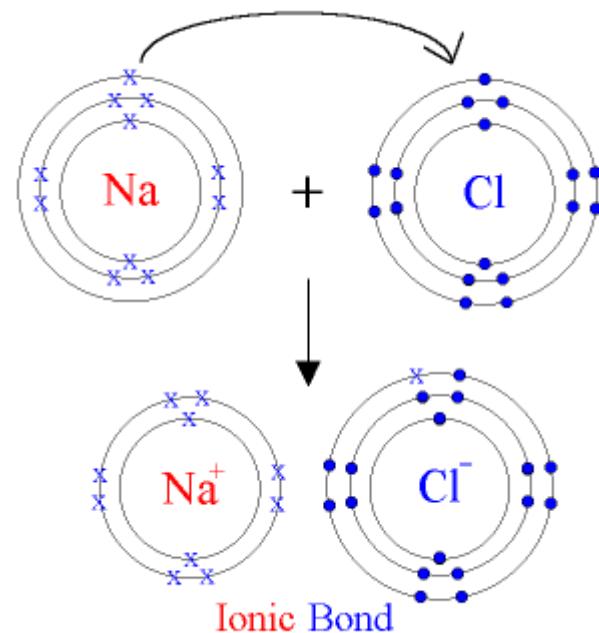


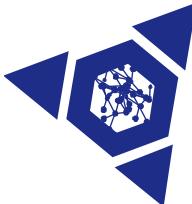
Ionic Bonds

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.





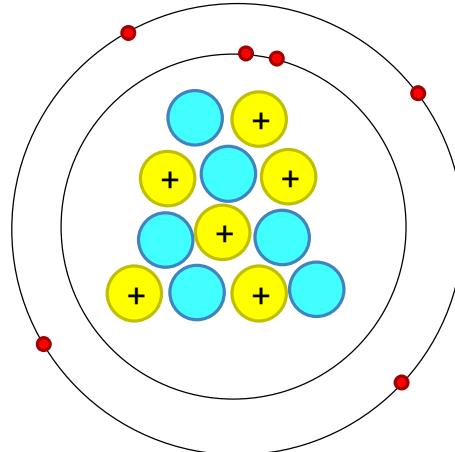
Covalent Bonding

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



Periodic Table of the Elements

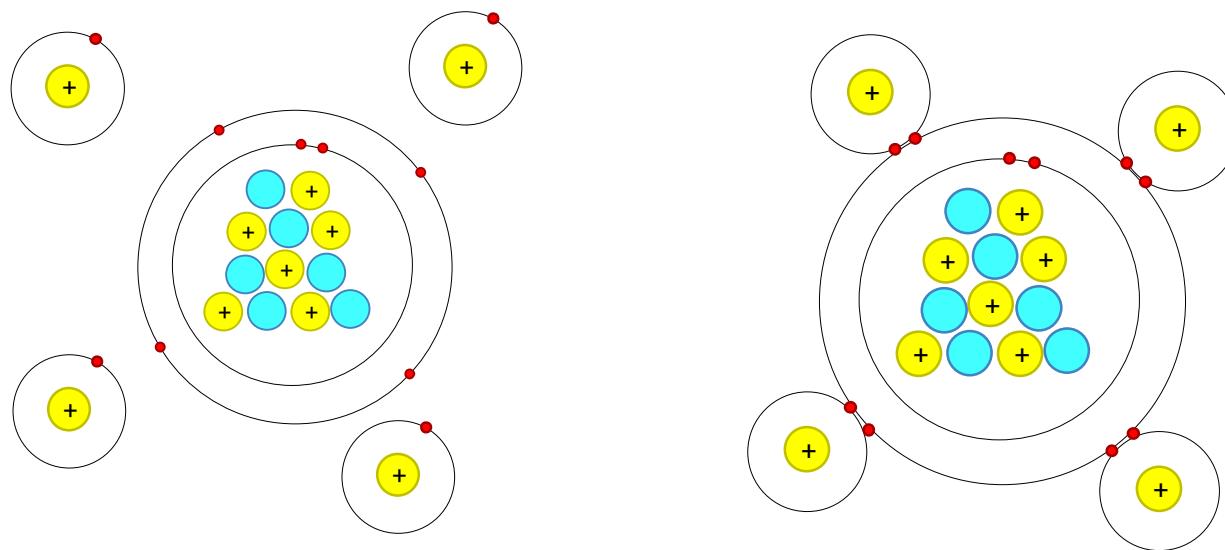
1	2	3	4	5	6	7	8	9	10
H									He
Li	Be								
Na	Mg								
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt
Fr	Ra	Ac	Unq	Unp	Unh	Uns	Uno	Uno	Unn
58	59	60	61	62	63	64	65	66	67
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es
90	91	92	93	94	95	96	97	98	99
104	105	106	107	108	109	110			
59	60	61	62	63	64	65	66	67	68
Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er
91	92	93	94	95	96	97	98	99	100
105	106	107	108	109	110				
61	62	63	64	65	66	67	68	69	70
Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
93	94	95	96	97	98	99	100	101	102
106	107	108	109	110					
63	64	65	66	67					
Eu	Gd	Tb	Dy	Ho					
95	96	97	98	99					
108	109	110							
64	65	66	67	68	69	70	71		
Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
96	97	98	99	100	101	102	103		



Electron Sharing, or Covalent Bonding

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

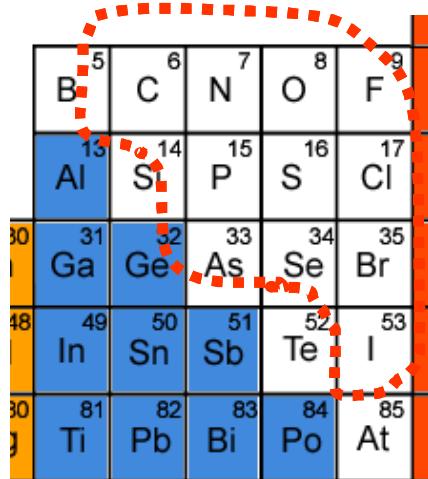
Four Hydrogen atoms can bond to one carbon atom:





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*

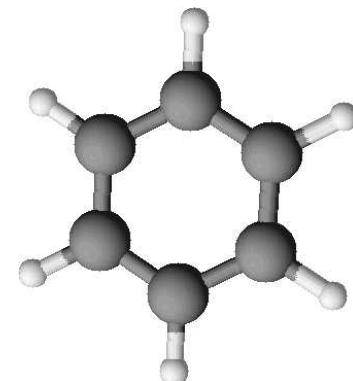
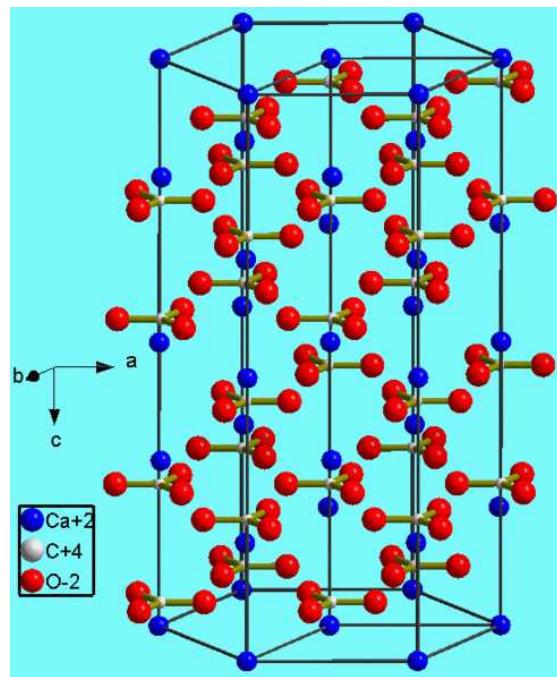




Compounds

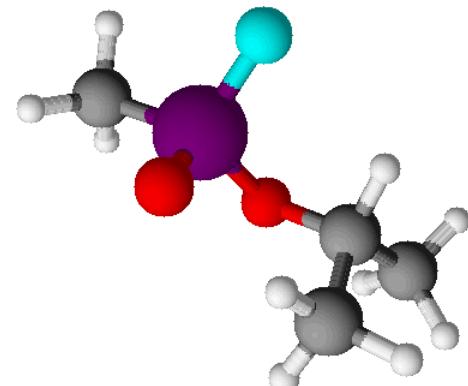
Chemical Compounds are composed of two or more chemical elements.

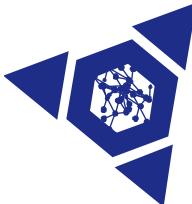
CaCO_3 , Calcium carbonate



C_6H_6 , Benzene

$\text{PO}_2\text{FC}_4\text{H}_{10}$, Sarin

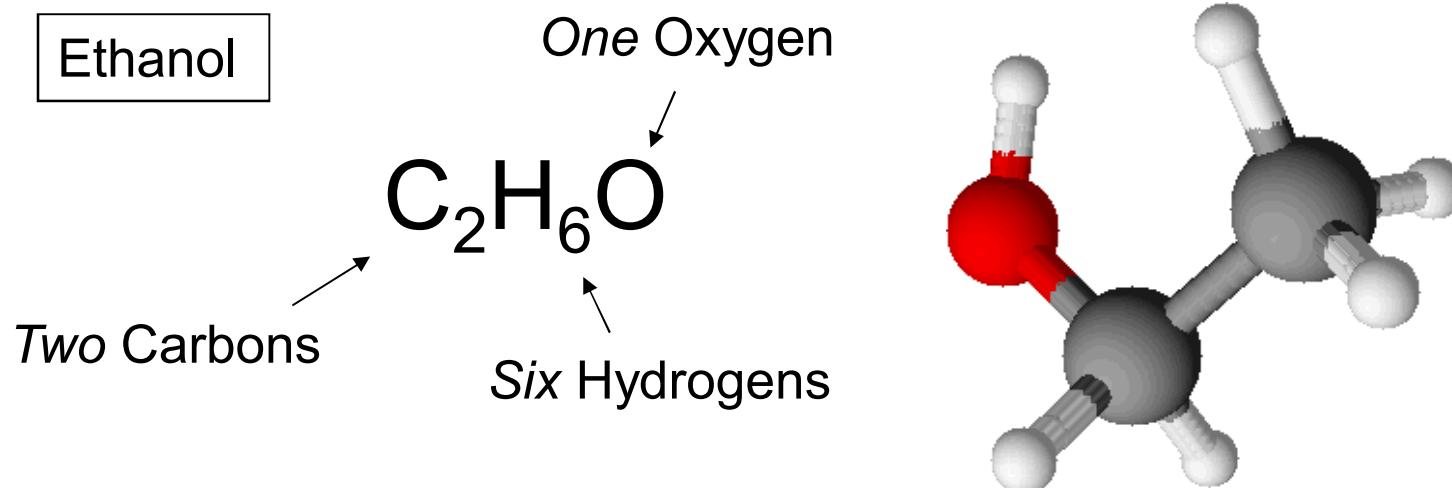




Chemical Formulas

Chemical Formulas are shorthand notation of composition.

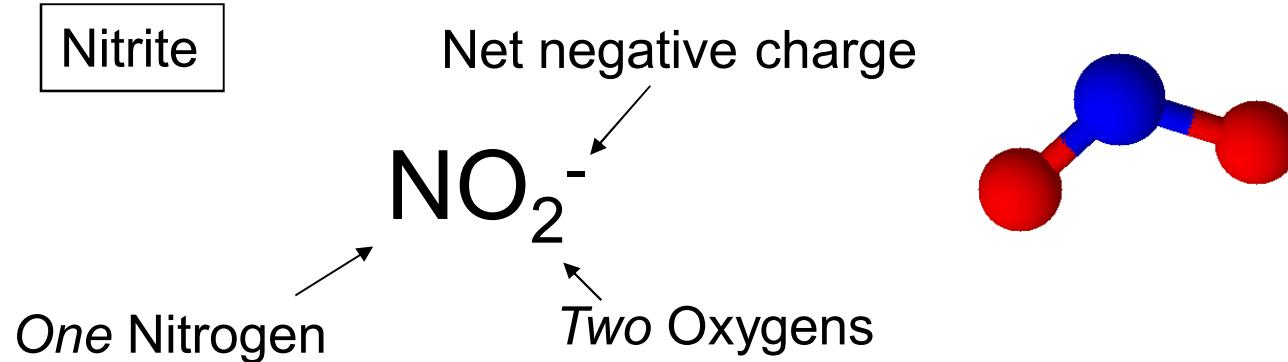
- Subscripts denote number of atoms.





Chemical Formulas

Chemical Formulas are shorthand notation of composition.

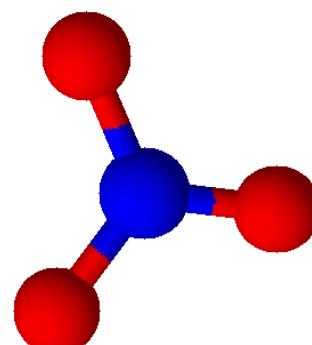
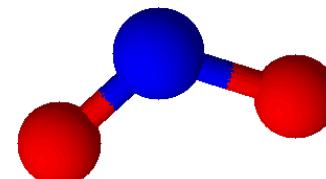




Oxidation States

- 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

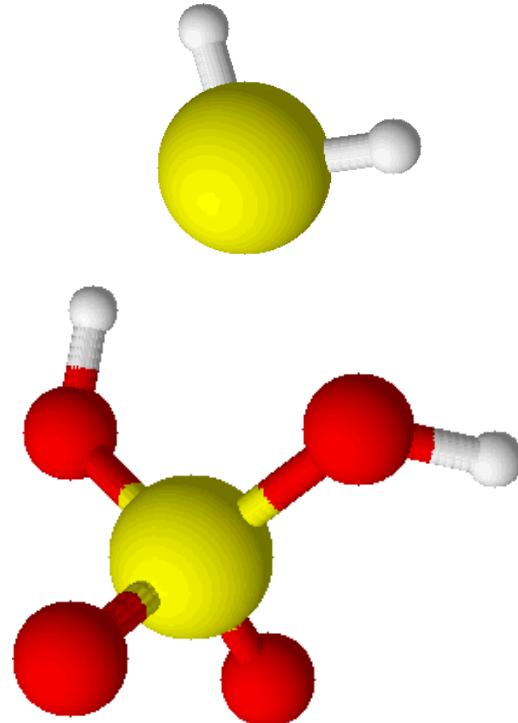


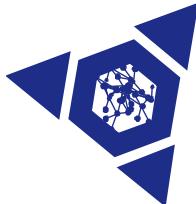


Oxidation States

- 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.

- 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:



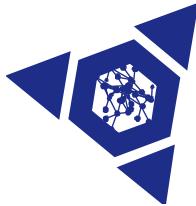
Charge on the nitrogen = net charge – (# of oxygens x -2)

Charge on the nitrogen = $(-1 - (2 \times -2))$

$$= (-1 - (-4))$$

$$= +3$$



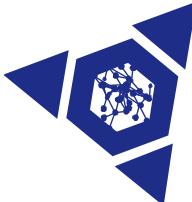


Oxidation States

Method to Determine Oxidation State of chlorine in perchlorate.

- 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 = $(-1 - (4 \times -2))$
 $= (-1 - (-8))$
 $= +7$

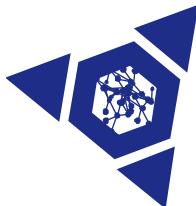




Flexible Oxidation States

Many main group atoms exhibit several oxidation 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

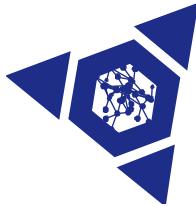
Pool chemical/muriatic acid reaction to generate chlorine gas.



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.