Mineral Chemistry

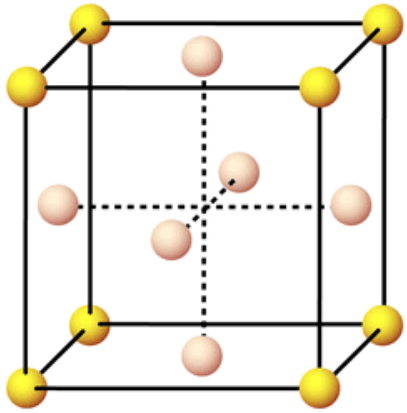
The chemical composition of a mineral is of fundamental importance. Many of mineral properties depend on its chemistry and its crystalline structure.

- Chemical analyses are usually reported in weight percent of elements or elemental oxides.
- To calculate mineral formula requires transforming weight percent into atomic percent or molecular percent.

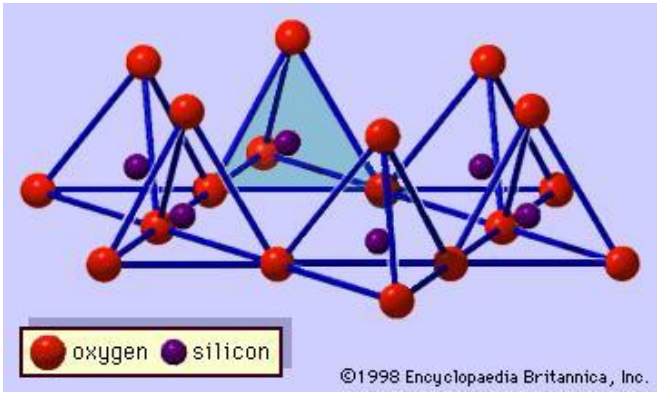
Elemental Mineral and Compound minerals:

- Elemental minerals are those naturally occurring minerals that are made up entirely of single elements from periodic table, such as Cupper (C), Sulfur (S), Kryptone (Kr), …. etc.

Cupper

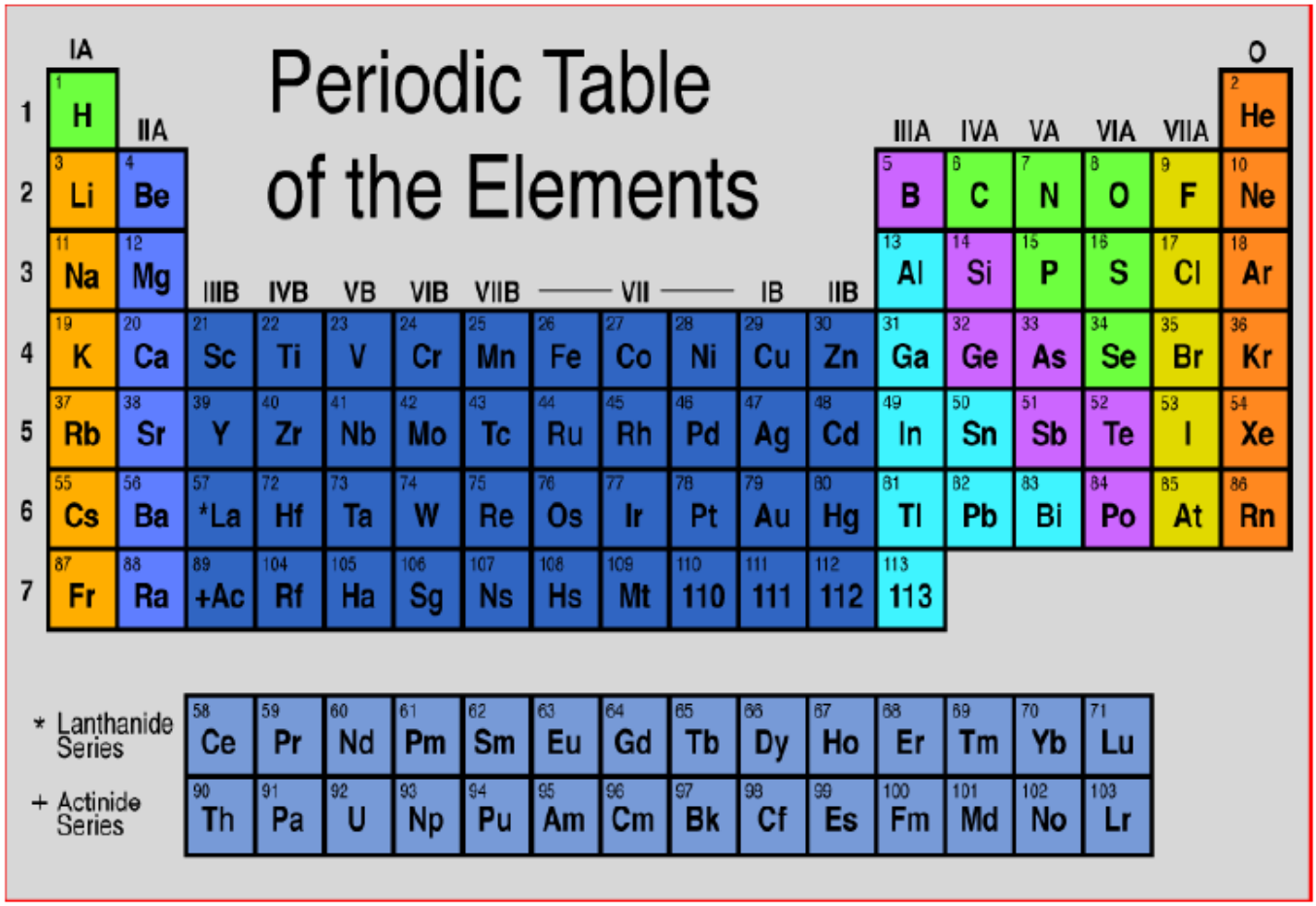


- Compound minerals are naturally occurring crystalline substance, which are formed by the chemical combination of two or more elements, such as silicate minerals such as quartz (SiO_2).



Basic terminology

- Atomic weight: tabulated in the periodic table of the elements (See table bellow).
- Molecular weight: weight of all the atoms in a given molecule.
  $H_2O = 2H + 1O = (2*1.00794) + (1*15.9994) = 18.01528$
- Mole: the amount of an element that has an equal weight to its atomic weight or Avogadro's Number (6.022 * 1023 atoms) of entities.
- Atoms per formula units (apfu): numbers of atoms in a chemical formula.



Mineral Chemistry Calculation:

The chemical compositions of minerals as reported in their chemical formulas are really ideal compositions based only on the proportions of their major element constituents, however minerals include minor and trace elements in their structure too.

- Major element are defined as any element occurring at >1% wt. in a mineral.
- Minor elements occurring at (1.0 – 0.1 % wt. abundance).
- Trace elements at (> 0.1% wt. İn abundance).

➢ Determination of Weight Percent (Wt%) of elements in a mineral:

The recuirements is :

1. chemical formula of a mineral.
2. Atomic weight of individual elements comprising mineral formula.
3. Chemical formulas are written with cation preceding anions; cations appear in order from left to right according to increasing valence.
4. İf the same valence exists for two or more cations, they can be written left to right according to alphabetic order of their chemical symbols.

Example: Calculate the Wt % of the elements in the Chalcopyrite mineral ($CuFeS_2$).

Elements	Atomic weight	Atoms / Formula	Molecular Weight Contribution	Wt % of Element
Cu	63.54	1	63.54	(63.54/183.51) x 100 = 34.62
Fe	55.85	1	55.85	(55.8/183.51) x 100 = 30.43
S	32.06	2	64.12	(64.1/183.51) x 100 = 34.94
Sum.			183.51	

➢ Determination of the chemical formula of a minerla:

The recuirements is :

1. Weight percent (Wt%) of each elements in the mineral.
2. Atomic weight of elements in the mineral.
3. Number of elemts atom calculations in the mineral.
4. Determination of the atomic proportions as bellow:

   The atomic proportion must be normalized dividing by the smallest number and rounded of to obtain the whole number.
5. Placing each appropriate subscript bellow the corresponding element in the formula will result in the chemical formula of the mineral ($CuFeS_2$).

Elements	Atomic weight	Weight %	Atomic Proportion	Subscript
Cu	63.54	34.62	(34.62/63.54) = 0.54	(0.54/0.54) = 1
Fe	55.85	30.43	(30.43/55.85) = 0.54	(0.54/0.54) = 1
S	32.06	34.94	(34.94/32.06) = 1.08	(1.08/0.54) = 2

Q1/ Calculate the percentage composition by weight of mineral Marcasite ftom the following data :

Elements	Atomic Weight
Fe	55.85
S	32.07

Note: Chemical formula of Marcasite is FeS_2

Q2/ From the following data determine the formula of Sphalerite mineral:

Elements	Weight %	Atomic Weights
Fe	18.36	55.84
Mn	2.68	54.93
Cd	0.28	112.41
Zn	44.92	65.38
S	33.76	32.06