BERKELEY MATH CIRCLE

The Math of Chemistry:

Chemical Reactions
&
Equilibrium

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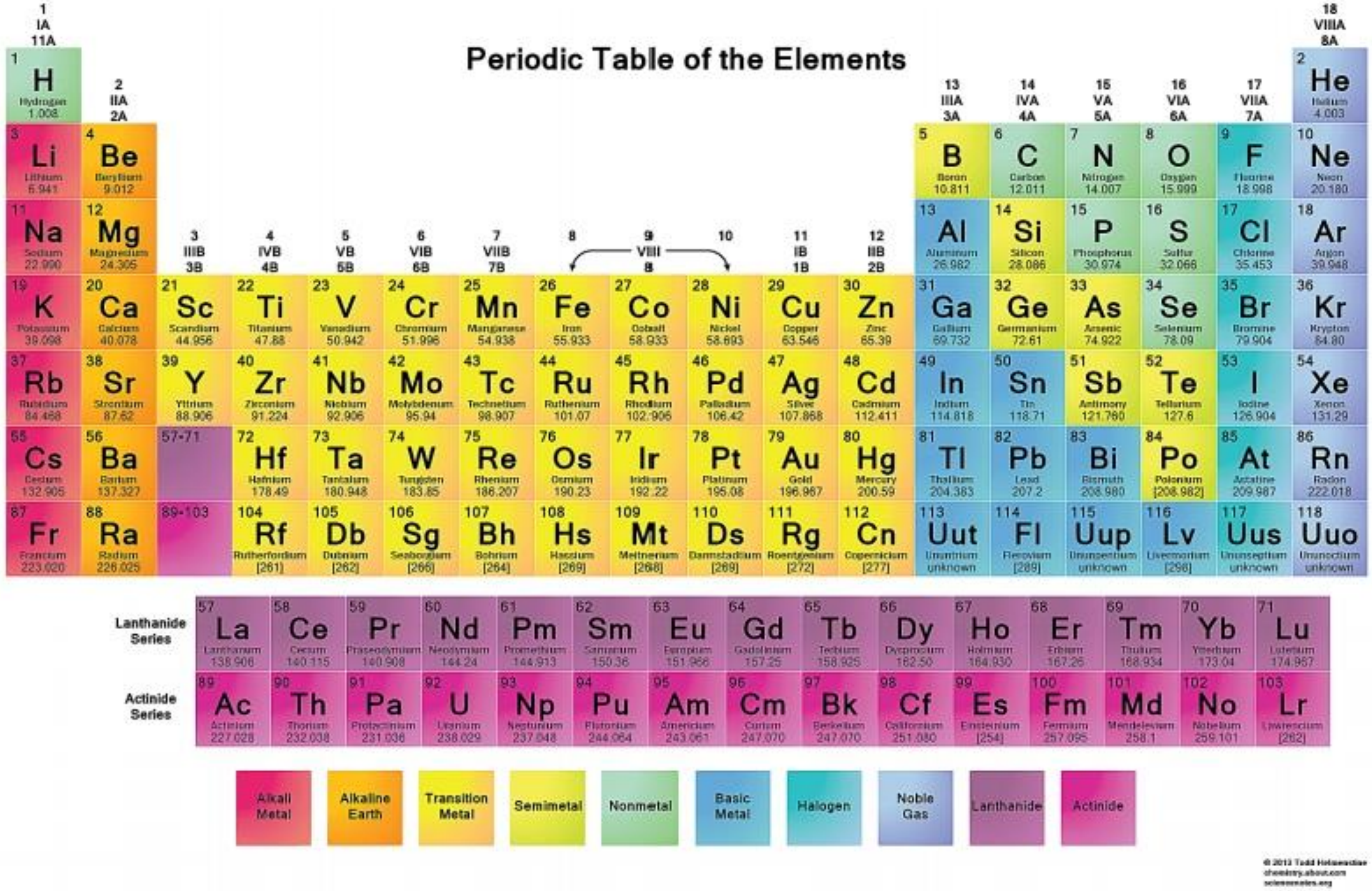
The Periodic Table



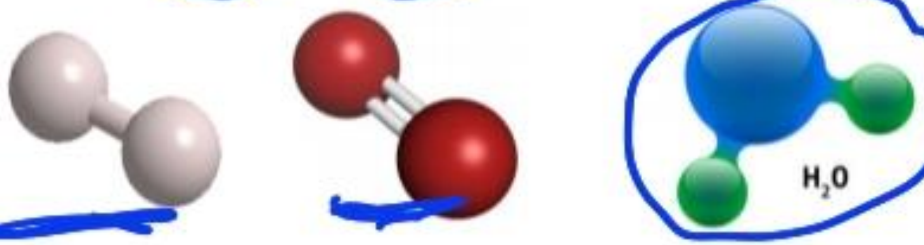
Chemical Reactions & Equilibrium

In Chemistry, we like to observe reactions as they happen. The reaction is considered to be done once it reaches what we call **Equilibrium**. At Equilibrium, the macroscopic reaction is done, but we do see things occurring on the microscopic level. For example,

Macroscopic

Microscopic

$$H_2 + O_2 \rightarrow H_2O$$



Chemical Reactions & Equilibrium

The reaction should continue until the reactants have been completely used up. However, this is not the case for most of the reactions because we have a **reverse reaction** taking place. Let us suppose that we begin our reaction by mixing two known reactants. At the beginning of the reaction, we have all the reactants and no products. As the reaction proceeds forward, the concentration of the reactants decreases. At the same time, the concentration of product begins to increase BUT some of the products begin to convert back to reactants.

Eventually the forward and backward reaction rates will be equal, and at this point we say that our reaction has reached dynamic chemical equilibrium.

$$H_2 + O_2 \rightleftarrows H_2O$$

Chemical Reactions & Equilibrium

We have a mathematical way to discuss this relationship, and that is referred to as the **Equilibrium Constant, K** (it's a fraction in essence, see below). The higher the equilibrium constant, the more products we have formed and the less reactants we have remaining. On the contrary, the smaller the equilibrium constant, the less product-favored our reaction, and the less product we have formed.

$$K = \frac{\text{products}}{\text{reactants}}$$

$$\text{reactants} \rightleftharpoons \text{products}$$

To do some math with this concept, we need to learn some fun background science-y things. Up first is learning how to balance chemical reactions. Here goes!

Chemical Reactions & Equilibrium

Balancing Chemical Reactions

The basic premise is that what goes in must come out, i.e., everything seen on the reactant side MUST also be seen on the product side. The forms of the molecules may have changed, but all the same atoms and the number of those atoms must be equal on both sides of the arrow. It's literally like an algebra equation!

For example:

$$PCl_3(g) + Cl_2(g) \rightleftarrows PCl_5(g)$$

We observe on the reactant side, that we have one P and five Cl's.

We see the same on the product side.

Chemical Reactions & Equilibrium

Balancing Chemical Reactions

SO_3 (g) $\rightleftarrows$ SO_2 (g) + O_2 (g) (not balanced)

On the reactant side, we have one S and three O's.
On the product side, we have one S and four O's.
We are not balanced!

$2SO_3$ (g) $\rightleftarrows$ $2SO_2$ (g) + O_2 (g) (balanced)

On the reactant side, we have two S's and six O's.
We now see the same on the product side.

Chemical Reactions & Equilibrium

Let's Practice Balancing Chemical Reactions!

$H_2 \quad + \quad O_2 \quad \rightleftarrows H_2O$

$N_2(g) \ + H_2(g) \ \rightleftharpoons NH_3(g)$

$CH_4(g) \ + O_2(g) \ \rightleftharpoons H_2O(g) \ + \ CO_2(g)$

Chemical Reactions & Equilibrium

Now that we know how to balance chemical equations, we can set-up our:

Equilibrium Constant (K)

Chemical reactions can be characterized by an **equilibrium constant,** K. This constant expresses the ratio of the product of the reaction products to the product of the reactants.

We use the concentrations (or pressures) of each molecule (those values are given or figured out per the word problem). The coefficient from the balanced chemical becomes the exponent for each term. So, for the reaction below, we have:

$$aA + bB \rightleftarrows cC + dD$$

$$K = \frac{\text{products}}{\text{reactants}} = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

Chemical Reactions & Equilibrium

From our previous reactions, we would have:

$2H_2 + O_2 \rightleftarrows 2H_2O$

$$K = \frac{prod}{react} = \frac{[H_2O]^2}{[H_2]^2[O_2]^1}$$

$N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g)$

$$K = \frac{[NH_3]^2}{[N_2][H_2]^3}$$

$CH_4(g) + 2O_2(g) \rightleftharpoons 2H_2O(g) + CO_2(g)$

$$K = \frac{[H_2O]^2 \cdot [CO_2]}{[CH_4] \cdot [O_2]^2}$$

Chemical Reactions & Equilibrium

Now, let's do some math with these chemical equations:

$$2H_2 + O_2 \rightleftarrows 2H_2O$$

$K = 3$

What is the equilibrium value for the above equation if we measured the following at equilibrium:

Hydrogen gas exhibits a partial pressure of 2 atm.
Oxygen gas exhibits a partial pressure of 3 atm.
Water vapor exhibits a partial pressure of 6 atm.

$[H_2]^2$

$$K = \frac{[H_2O]^2}{[H_2]^2[O_2]} = \frac{6^2}{2^2 \cdot 3} = \frac{36}{4 \cdot 3} = \frac{36}{12} = 3$$

Chemical Reactions & Equilibrium

Using the same chemical equation,

$$2H_2 + O_2 \rightleftarrows 2H_2O$$

$K = 3$

17 atm H_2O

1) What is the water vapor's pressure at equilibrium if we ~~started~~ ended with 4 atm of hydrogen gas and 3 atm of Oxygen gas?

$$K = \frac{[H_2O]^2}{[H_2]^2[O_2]} \Rightarrow 3 = \frac{x^2}{4^2 \cdot 3}$$

~~2) What is the hydrogen's pressure at equilibrium if we started with 3 atm of water vapor and 1/3 atm of oxygen gas?~~

$$3 = \frac{x^2}{4^2 \cdot 3} \Rightarrow x^2 = 3^2 \cdot 4^2 \stackrel{\sqrt{}}{\Rightarrow} x = 3 \cdot 4 = 12$$

Chemical Reactions & Equilibrium

$$3 \cdot 4^2 \quad 3 = \frac{x^2}{3 \cdot 4^2} \quad \times 3 \cdot 4^2$$

$$3 \cdot 4^2 \cdot 3 = x^2$$

$$144 = x^2 \Rightarrow \sqrt{x^2} = \sqrt{144}$$

$$x = 12$$