BERKELEY MATH CIRCLE

The Math of Chemistry:

Chemical Reactions
&
Equilibrium

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The Periodic Table

Periodic Table of the Elements

1 IA 11A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8	9 VIII 8	10	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A
1 H Hydrogen 1.008																	2 He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.88	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.933	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.732	32 Ge Germanium 72.61	33 As Arsenic 74.922	34 Se Selenium 78.09	35 Br Bromine 79.904	36 Kr Krypton 84.80
37 Rb Rubidium 84.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.29
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.85	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987	86 Rn Radon 222.018
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103	104 Rf Rutherfordium [261]	105 Db Dubnium [262]	106 Sg Seaborgium [266]	107 Bh Bohrium [264]	108 Hs Hassium [269]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [269]	111 Rg Roentgenium [272]	112 Cn Copernicium [277]	113 Uut Ununtrium unknown	114 Fl Flerovium [289]	115 Uup Ununpentium unknown	116 Lv Livermorium [298]	117 Uus Ununseptium unknown	118 Uuo Ununoctium unknown

Lanthanide Series	57 La Lanthanum 138.906	58 Ce Cerium 140.115	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.24	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.966	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.50	67 Ho Holmium 164.930	68 Er Erbium 167.26	69 Tm Thulium 168.934	70 Yb Ytterbium 173.04	71 Lu Lutetium 174.967
Actinide Series	89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium [254]	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium [262]

Alkali Metal	Alkaline Earth	Transition Metal	Semimetal	Nonmetal	Basic Metal	Halogen	Noble Gas	Lanthanide	Actinide

Chemical Reactions & Equilibrium

Equilibrium Constant (K)

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

K is a CONSTANT, which means it is always the same value for a given chemical reaction under like conditions (temp, pressure, etc.). So, once you know the value K for a reaction, it applies always to that reaction under like conditions!

For rxn:

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

K = products / reactants $= \frac{[C]^c[D]^d}{[A]^a[B]^b}$ → amounts of substances

Chemical Reactions & Equilibrium

For this equation:

$C_6H_{12}O_6 + 6O_2 \rightleftharpoons 6H_2O + 6CO_2$

Glucose

18 O's

18 O's

1) Write out a balanced chemical equation (remember our useful rule of thumb!)

2) Find the K value if at equilibrium the following is observed:

$[C_6H_{12}O_6] = 0.5M$
$[O_2] = 3M$
$[H_2O] = 2M$
$[CO_2] = 3M$

$$K = \frac{[H_2O]^6[CO_2]^6}{[C_6H_{12}O_6][O_2]^6} = \frac{(2)^6(3)^6}{(0.5)(3)^6}$$

$$\frac{2^6}{1/2} = 2^6 \div \frac{1}{2} = 2^6 \times 2 = 2^7 = 128$$

Chemical Reactions & Equilibrium

For this equation:

$$C_6H_{12}O_6 + 6O_2 \rightleftharpoons 6H_2O + 6CO_2$$

$K = 128$

#3

Find the concentration of glucose if at equilibrium the following is measured:

$[O_2] = 2M$
$[H_2O] = 4M$
$[CO_2] = 2M$

$$K = \frac{[H_2O]^6[CO_2]^6}{[C_6H_{12}O_6][O_2]^6} \Rightarrow 128 = \frac{(4)^6(2)^6}{(a)(2)^6}$$

$$\frac{128}{1} = \frac{4^6}{a}$$

$$128a = 4^6 \quad (\div 128)$$

$$a = \frac{4^6}{128} = \frac{(2^2)^6}{2^7} = \frac{2^{12}}{2^7}$$

$$a = \frac{2^{12}}{2^7} = 2^5$$

$$a = 32$$

Chemical Reactions & Equilibrium

Now, what if we can look at a reaction WHILE it is occurring, and before it is finished? How does this compare with our equilibrium concept, and the Equilibrium Constant?

If we took a snapshot of our reaction and measure the amounts of the substances in use, we can still set-up the equation for the equilibrium value, BUT, since it is not yet at equilibrium, we can't call it K. Instead, we call it Q, which is EXACTLY the same fraction set-up as before, but Q is when the reaction is in progress.

From before, for this reaction, aA + bB ⇄ cC + dD, we have:

$$K = \frac{prod}{react} = \frac{C^c \cdot D^d}{A^a \cdot B^b} \qquad Q = \frac{prod}{react} = \frac{C^c \cdot D^d}{A^a \cdot B^b}$$

Let's learn this via an example!

Chemical Reactions & Equilibrium

Let's use this equation as our chemical reaction (decomposition of Nitric Oxide):

$$2NO \rightleftarrows N_2 + O_2$$

Assuming equilibrium values of the following, find K.

$NO = 1.0$ atm
$N_2 = 1.0$ atm
$O_2 = 1.0$ atm

$$K = \frac{(N_2)(O_2)}{(NO)^2} = \frac{(1)(1)}{(1)^2} = \frac{1}{1} = 1$$

Chemical Reactions & Equilibrium

Let's use this equation as our chemical reaction:

$$2NO \rightleftarrows N_2 + O_2$$

Assuming equilibrium values of the following, find K.

$NO = 1.0$ atm
$N_2 = 1.0$ atm
$O_2 = 1.0$ atm

$K = [O_2][N_2] / [NO]^2 = [1.0]\,[1.0] / [1.0]^2 = 1.0$

$K = 1$

Chemical Reactions & Equilibrium

$K = \frac{(N_2)(O_2)}{(NO)^2}$

$$2NO \rightleftarrows N_2 + O_2$$

$K = 1$

We know that the equilibrium value, K, is 1.0 for this reaction.
Let's now compare two new sets of measurements for this reaction:

Measurement Set #1
NO = 4.0 atm
N_2 = 1.0 atm
O_2 = 1.0 atm

$Q = \frac{(1)(1)}{4^2} = \frac{1}{16} = 0.0625$

Measurement Set #2
NO = 1.0 atm
N_2 = 2.0 atm
O_2 = 2.0 atm

$Q = \frac{2 \cdot 2}{1^2} = \frac{4}{1} = 4$

Chemical Reactions & Equilibrium

$$2NO \rightleftarrows N_2 + O_2$$

So what does this all mean?

Mathematically, we have three scenarios:

$Q < K$

$Q = K$

$Q > K$

$$K = \frac{prod}{react} = \frac{num}{denom}$$

Scientifically (i.e., reaction-wise), we have:

$Q < K$ means not enough of the reaction has happened, and the rxn needs to adjust

$Q = K$ means the reaction is done

$Q > K$ means too much of the reaction has happened, and the rxn to adjust

BONUS Question: How do we know which way our rxn adjusts?

Chemical Reactions & Equilibrium

Going back to our new measurement sets, what do we expect to occur?

Measurement Set #1

NO = 4.0 atm

N_2 = 1.0 atm

O_2 = 1.0 atm

$K = [O_2][N_2] / [NO]^2 = [1.0]\,[1.0] / [4.0]^2 = 1/16 = 0.0625 < 1.0$

Measurement Set #2

NO = 1.0 atm

N_2 = 2.0 atm

O_2 = 2.0 atm

$K = [O_2][N_2] / [NO]^2 = [2.0]\,[2.0] / [1.0]^2 = 4 > 1.0$

Chemical Reactions & Equilibrium

And the million dollar question is how do we determine the new equilibrium values?

$$2NO \rightleftarrows N_2 + O_2$$

We use ICE!

I = Initial
C = Change
E = Equilibrium

Using the balanced chemical equation, we set up a table using the concentrations we know, and the ones we don't know we use variables. Then we tackle the math with ALGEBRA!

BONUS Question: How do we know which way our rxn adjusts?

Chemical Reactions & Equilibrium

	$2NO$ ⇌	N_2 +	O_2
I = Initial			
C = Change			
E = Equilibrium			

Chemical Reactions & Equilibrium

	$2NO$	N_2	O_2
I = Initial	4	1	1
C = Change	$-2x$	$+x$	$+x$
E = Equilibrium	$4-2x$	$1+x$	$1+x$

Measurement Set #1

NO = 4.0 atm

N_2 = 1.0 atm

O_2 = 1.0 atm

$K = [O_2][N_2] / [NO]^2 = [1.0][1.0] / [4.0]^2 = 1/16 = 0.0625 < 1.0$

Chemical Reactions & Equilibrium

	2NO	N_2	O_2
I = Initial	4.0	1.0	1.0
C = Change	- 2x	+ x	+ x
E = Equilibrium	4 – 2x = 2	1 + x = 2	1 + x = 2

Measurement Set #1
NO = 4.0 atm
N_2 = 1.0 atm
O_2 = 1.0 atm

$K = [O_2][N_2] / [NO]^2 = [1.0][1.0] / [2.0]^2 = 1/4 = 0.25 < 1.0$

$$K = 1 = \frac{(1+x)(1+x)}{(4-2x)^2} \Rightarrow 1 = \frac{1+x}{4-2x}$$

$$4-2x = 1+x$$
$$3 = 3x$$
$$x = 1$$