

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

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

Alkali Metal	Alkaline Earth	Transition Metal	Semimetal	Nonmetal	Basic Metal	Halogen	Noble Gas	Lanthanide	Actinide
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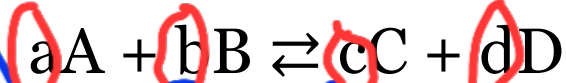
# Chemical Reactions & Equilibrium

## 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:



K =

products  
reactants

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

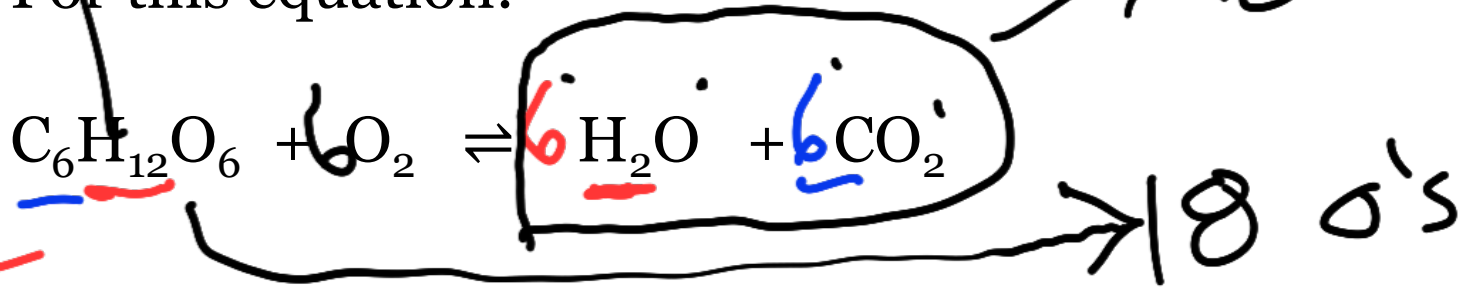
amounts of substances

coefficients

Glucose

# Chemical Reactions & Equilibrium

For this equation:



$$\frac{2^6}{4^7} = 2^6 \div \frac{1}{2}$$
$$= 2^6 \times 2$$
$$= 2^7 = \boxed{128}$$

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

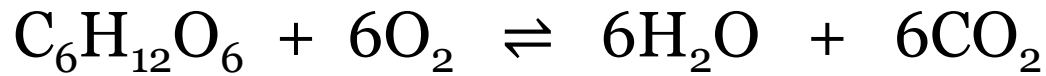
2) Find the K value if at equilibrium the following is observed:

$$[\text{C}_6\text{H}_{12}\text{O}_6] = 0.5\text{M}$$
$$[\text{O}_2] = 3\text{M}$$
$$[\text{H}_2\text{O}] = 2\text{M}$$
$$[\text{CO}_2] = 3\text{M}$$

$$K = \frac{[\text{H}_2\text{O}]^6 [\text{CO}_2]^6}{[\text{C}_6\text{H}_{12}\text{O}_6] [\text{O}_2]^6} = \frac{(2)^6 (3)^6}{(0.5) (3)^6}$$

# Chemical Reactions & Equilibrium

For this equation:



$$K = 128$$

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

$a = 32$

#3

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

$$\begin{aligned} [\text{O}_2] &= 2\text{M} \\ [\text{H}_2\text{O}] &= 4\text{M} \\ [\text{CO}_2] &= 2\text{M} \end{aligned}$$

$$K = \frac{[\text{H}_2\text{O}]^6 [\text{CO}_2]^6}{[\text{C}_6\text{H}_{12}\text{O}_6] [\text{O}_2]^6}$$

$$\Rightarrow 128 = \frac{(4)^6 (\cancel{2})^6}{(a) (\cancel{2})^6}$$

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

$\frac{1}{128} \quad \frac{1}{128}$

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

# 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,  $aA + bB \rightleftharpoons cC + dD$ , we have:

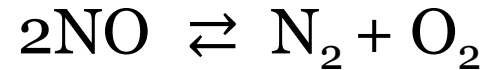
$$K = \frac{\text{prod}}{\text{react}} = \frac{C^c \cdot D^d}{A^a \cdot B^b} \qquad Q = \frac{\text{prod}}{\text{react}} = \frac{C^c \cdot D^d}{A^a \cdot B^b}$$

Let's learn this via an example!



# Chemical Reactions & Equilibrium

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



Assuming equilibrium values of the following, find K.

NO = 1.0 atm

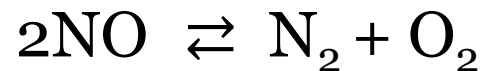
N<sub>2</sub> = 1.0 atm

O<sub>2</sub> = 1.0 atm

$$K = \frac{(\text{N}_2)(\text{O}_2)}{(\text{NO})^2} = \frac{(1)(1)}{(1)^2} = \frac{1}{1} = 1$$

# Chemical Reactions & Equilibrium

Let's use this equation as our chemical reaction:



Assuming equilibrium values of the following, find K.

$$\text{NO} = 1.0 \text{ atm}$$

$$\text{N}_2 = 1.0 \text{ atm}$$

$$\text{O}_2 = 1.0 \text{ atm}$$

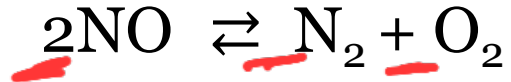
$$K = \frac{[\text{O}_2][\text{N}_2]}{[\text{NO}]^2} = \frac{[1.0][1.0]}{[1.0]^2} = 1.0$$

$$K = 1$$



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

# Chemical Reactions & Equilibrium



$$K = 1$$

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

$$NO = 4.0 \text{ atm}$$

$$N_2 = 1.0 \text{ atm}$$

$$O_2 = 1.0 \text{ atm}$$

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

## Measurement Set #2

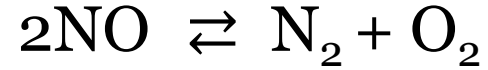
$$NO = 1.0 \text{ atm}$$

$$N_2 = 2.0 \text{ atm}$$

$$O_2 = 2.0 \text{ atm}$$

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

# Chemical Reactions & Equilibrium



So what does this all mean?

Mathematically, we have three scenarios:

$$Q < K$$

$$Q = K$$

$$Q > K$$

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

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

$$\text{NO} = 4.0 \text{ atm}$$

$$\text{N}_2 = 1.0 \text{ atm}$$

$$\text{O}_2 = 1.0 \text{ atm}$$

$$K = [\text{O}_2][\text{N}_2] / [\text{NO}]^2 = [1.0][1.0] / [4.0]^2 = 1/16 = 0.0625 < 1.0$$

## Measurement Set #2

$$\text{NO} = 1.0 \text{ atm}$$

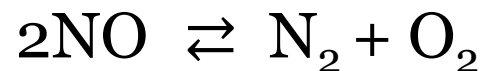
$$\text{N}_2 = 2.0 \text{ atm}$$

$$\text{O}_2 = 2.0 \text{ atm}$$

$$K = [\text{O}_2][\text{N}_2] / [\text{NO}]^2 = [2.0][2.0] / [1.0]^2 = 4 > 1.0$$

# Chemical Reactions & Equilibrium

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



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

	$2\text{NO}$		$\text{N}_2$	$+$	$\text{O}_2$
<b>I = Initial</b>					
<b>C = Change</b>					
<b>E = Equilibrium</b>					

# Chemical Reactions & Equilibrium

	$2\text{NO}$	$\rightleftharpoons$	$\text{N}_2$	+	$\text{O}_2$
<b>I = Initial</b>					
<b>C = Change</b>	$-2x$		$+x$		$+x$
<b>E = Equilibrium</b>	$4 - 2x$		$1 + x$		$1 + x$

**Measurement Set #1**  
 $\text{NO} = 4.0 \text{ atm}$   
 $\text{N}_2 = 1.0 \text{ atm}$   
 $\text{O}_2 = 1.0 \text{ atm}$

$$K = [\text{O}_2][\text{N}_2] / [\text{NO}]^2 = [1.0][1.0] / [4.0]^2 = 1/16 = 0.0625 < 1.0$$

# Chemical Reactions & Equilibrium

	2NO	N <sub>2</sub>	O <sub>2</sub>
<b>I = Initial</b>	4.0	1.0	1.0
<b>C = Change</b>	- 2X	+ X	+ X
<b>E = Equilibrium</b>	4 - 2X = 2	1 + X = 2	1 + X = 2

## Measurement Set #1

NO = 4.0 atm

N<sub>2</sub> = 1.0 atm

O<sub>2</sub> = 1.0 atm

$$K = [\text{O}_2][\text{N}_2] / [\text{NO}]^2 = [1.0][1.0] / [2.0]^2 = 1/4 = 0.25 < 1.0$$

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

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

$$3 = 3x$$

$$x = 1$$