Chemical Reactions

Themes for this subject:
1. If a system, molecule, or ionic compound is not stable, how will it change to become more stable?
2. The answer to question #1 is quite dependent on the specific environmental surroundings of the system, molecule, etc.
3. We will not be able to reach completely satisfying answers to all of your questions on this subject, but try to master the basic patterns.

Look at an example: Rxn. of Cu\(^{2+}\) (from CuCl\(_2\)) with Al (demo):

Write an equation describing the rxn.: 

\[
\text{________ + _______} \rightarrow \text{________ + _______}
\]

\[
\text{________ + _______} \rightarrow \text{________ + _______}
\]

I. What is a chemical change & how do we describe it?
A. This is simple if we are looking at covalent compounds: Any change involving forming or breaking covalent bonds is a chemical change.

1. Example: Rxn. of hydrogen and oxygen to form water:

chemical equation: \[2 \text{H}_2(g) + \text{O}_2(g) \rightarrow 2 \text{H}_2\text{O}(g)\] (States: s.l.g,aq)

structurally expanded:

The old single bonds between the H atoms and the double bonds between the O atoms are broken and new single bonds between the H and O atoms are formed. This is a chemical reaction or chemical change (as opposed to physical change).
2. Would evaporation of water, $\text{H}_2\text{O}(l) \rightarrow \text{H}_2\text{O}(g)$, be a chemical change? Y or N
   If no, what type of change is this? ________________
   (A phase change is a physical change.)

3. Would dissolving glucose (a sugar) in tea, $\text{C}_6\text{H}_{12}\text{O}_6(s) \rightarrow \text{C}_6\text{H}_{12}\text{O}_6(aq)$
   be a chemical change? Y or N
   If no, what type of change is this? ________________

B. The picture is a little more complex when we look at ionic compounds

1. Is NaCl dissolving in water, NaCl(s) $\rightarrow$ NaCl(aq) a chemical change?
   Y or N
   This is a gray area. Ionic bonds in the salt (NaCl(s)) are broken when the salt
   dissolves. New interactions form between individual Na$^+$ and Cl$^-$ ions &
   H$_2$O when the aqueous solution ((aq)) forms. But the ions are not changed
   when they are dissolved, and if the water is evaporated, you get the NaCl
   crystals back.

2. Is NaCl melting, NaCl(s) $\rightarrow$ NaCl(l) a chemical change? Y or N
   No. Though a given Na$^+(l)$ may interact w/ a different set of Cl$^-$ ions than it
   was in the (s) state, it is still interacting with Cl$^-$ ions.

3. Is reaction of ionic copper II (Cu$^{2+}$(aq)) with elemental aluminum (Al (s)) a
   chemical change? Y or N
   Expand your thoughts? ________________

Aside: Balancing equations

1. A balanced equation has the same number of atoms of each element on the product side
   as on the reactant side. Charge must also be conserved.

2. You must determine the correct molecular/ionic formulas of the products before
   balancing.

3. There are a number of ways to balance equations. The elements can be balanced in
   any order, although some ways are much more efficient than others.
   Coefficients (whole numbers placed in front of each substance) are used to balance an equation.
   The coefficient applies to each element present in the substance.
   For example: 3 CuCl$_2$ means 3 Cu$^{2+}$ions and 6 Cl$^-$ ions.
Going back to the reaction at the beginning of these notes:

Full equation (unbalanced): \( \text{CuCl}_2 (aq) + \text{Al} (s) \rightarrow \text{Cu} (s) + \text{AlCl}_3 (aq) \)

How do you know that reaction is not balanced? _______________

Balance Cl, by realizing that \( 2 \times 3 = 6 \), so

\[ 3 \text{CuCl}_2 (aq) + \text{Al} (s) \rightarrow \text{Cu} (s) + 2 \text{AlCl}_3 (aq) \]

Now balance the Al with a 2, and Cu with a 3.

\[ 3 \text{CuCl}_2 (aq) + 2 \text{Al} (s) \rightarrow 3 \text{Cu} (s) + 2 \text{AlCl}_3 (aq) \]

Net ionic equation (unbalanced): \( \text{Cu}^{2+}(aq) + \text{Al} (s) \rightarrow \text{Cu} (s) + \text{Al}^{3+}(aq) \)

How do you know that reaction is not balanced? _______________

What is the best way to balance it? Half-reactions are one approach:

\[ \text{Cu}^{2+}(aq) + 2e^- \rightarrow \text{Cu} (s) \]

\[ \text{Al} (s) \rightarrow 3e^- + \text{Al}^{3+}(aq) \]

You need to have the same number of electrons on each side, so multiply the copper equation by 3 and the aluminum equation by 2:

\[
3 \text{Cu}^{2+}(aq) + 6e^- \rightarrow 3 \text{Cu} (s) \\
+ 2 \text{Al} (s) \rightarrow 6e^- + 2 \text{Al}^{3+}(aq)
\]

sum: \( 3 \text{Cu}^{2+}(aq) + 2 \text{Al} (s) + 6e^- \rightarrow 3 \text{Cu} (s) + 2 \text{Al}^{3+}(aq) + 6e^- \)

You can now cancel out the \( e^- \).

Balanced net ionic equation: \( 3 \text{Cu}^{2+}(aq) + 2 \text{Al} (s) \rightarrow 3 \text{Cu} (s) + 2 \text{Al}^{3+}(aq) \)

4. Benefits of each type of equation:
5. Finally, writing the balanced net ionic equation, starting from balanced full equation.

a) Starting from:
\[ 3 \text{CuCl}_2(aq) + 2 \text{Al}(s) \rightarrow 3 \text{Cu}(s) + 2 \text{AlCl}_3(aq) \]

b) Any species that is (s), (l) or (g) and any covalent compound that is (aq) in a full balanced equation, is unchanged in the net ionic equation. For ionic compounds that are (aq), the ions must be written separately in the ionic equation. In this case, CuCl\(_2\) and AlCl\(_3\) are written as the sum of their ions.

\[ 3 \text{Cu}^{2+}(aq) + 6 \text{Cl}^- (aq) + 2 \text{Al}(s) \rightarrow 3 \text{Cu}(s) + 2 \text{Al}^{3+}(aq) + 6 \text{Cl}^- (aq) \]

c) Realize that the Cl\(^-\) ions are just sitting around in the solution “doing nothing”; they are just spectating (watching). Ions not involved in the actual equation are called “spectator” ions. Any spectator ions (unchanged from reactant side to product side) are cancelled.

Balanced net ionic equation: \[ 3 \text{Cu}^{2+}(aq) + 2 \text{Al}(s) \rightarrow 3 \text{Cu}(s) + 2 \text{Al}^{3+}(aq) \]

6. Another example: Balance the following equation, then write the net ionic equation.

\[ \text{HNO}_3(aq) + \text{Mg(OH)}_2(s) \rightarrow \text{Mg(NO}_3)_2(aq) + \text{H}_2\text{O}(l) \]

II. Is it easier to understand reactions if we classify them?

\textbf{Yes!!!} There are millions of chemical rxns. If don’t put them into categories, there is no way we can keep track of them.

A. General chemistry categories:

1. \textbf{Combination} rxns.: \( A + B \rightarrow AB \)

This is two separate species coming together to form one compound:
Mg(s) + F₂(g) → MgF₂(s) \hspace{1cm} \textit{Too dangerous to demonstrate!}

For this eq, the net ionic eq is the same as balanced eq.

2. **Decomposition rxns.**: AB → A + B

Here, one species is falling apart (decomposing) to give 2 or more products.

Dehydrogenation (removal of H from) ethane is an example:

![Ethane and Ethene](image)

3. **Replacement rxns**
   - **a) Single replacement rxns.**: A + BC → B + AC

     \[ 2\text{Al}(s) + 3\text{CuCl}_2(aq) \rightarrow 3\text{Cu}(s) + 2\text{AlCl}_3(aq) \]

     Is the net ionic equation the same as the balanced equation? ______
     What would the net ionic equation be?

   - **b) Double replacement rxns.**: AB + CD → AD + CB

     i) Let’s look at the rxn. of CaCl₂(aq) with Na₂CO₃(aq):

     \[ \text{CaCl}_2(aq) + \text{Na}_2\text{CO}_3(aq) \rightarrow \text{CaCO}_3(s) + 2 \text{NaCl}(aq) \]

     What 2 ions are spectator ions? __________ & __________
     To answer this you must be able to picture (aq) in your mind.

     Can you write a net ionic equation for this rxn?

     ii) Acid-base neutralization reactions. (Key: H⁺ and OH⁻)

     \[ \text{HCl}(aq) + \text{KOH}(aq) \rightarrow \text{________} + \text{________} \]

4. **Combustion**

     __CH₄ + ___ O₂ → __________ + __________

   a) What are the products (when oxygen is in excess)?
b) Balance.
c) Does your car/motorcycle/yacht run any rxns like this?
d) Does your body run any reactions like this?

B. Comments on oxidation-reduction (redox) reactions.
1. By definition:
   a) Oxidation occurs when an atom, ion, or molecule:
      i) loses $e^-$
      ii) loses H atom equivalents
      iii) gains oxygen
   b) Reduction occurs when an atom, ion, or molecule:
      i) gains $e^-$
      ii) gains H atom equivalents
      iii) loses oxygen

2. All S.R. reactions, some synthesis and some decomposition reactions are oxidation/reduction reactions.

3. If you can keep track of $e^-$, H atom equivalents, and O, it will be easier for you to understand bunches of chemistry (batteries, corrosion, hemoglobin function, and energy metabolism, etc.).

4. The oxidation state of a compound often alters its function.
   For example: Hemoglobin (Hb) carries O$_2$ efficiently when its heme Fe is in the $+2$ oxidation state (Fe$^{2+}$), but not in the $+3$ state.

Hemoglobin (Hb):
pdb code: 1a3n

1. Hb is a tetramer ($\alpha_2\beta_2$).

2. Each of the 4 subunits contains one heme.

3. The hemes are flat structures.
   (For the light blue subunit, the heme is shown in sea-foam green.)

4. O$_2$ binds to the Fe$^{2+}$, which is at the center of each heme.
We live in an oxidizing environment. (There is lots of O\(_2\) around.) If the Fe in the heme is oxidized from +2 to +3, the resulting Hb is called methemoglobin (metHb). It is not an effective carrier of O\(_2\)

\[
\text{Hb(Fe}^{2+}\text{) } \rightarrow \text{ metHb(Fe}^{3+}\text{) } + e^{-}
\]

Losing just one \(e^-\) can make a big difference:

5. There are several disease states that exist because a patient has problems with the oxidation state of their Hb(Fe).


6. One way occurs due to a mutation in the beta (\(\beta\)) chain of Hb that makes the heme Fe more readily oxidized. (Hb has 2 \(\alpha\) & 2 \(\beta\) chains.) This condition is called hemoglobin M disease.

See:

7. Your Hb(Fe) is occasionally oxidized to the Fe$^{3+}$ when it releases oxygen. You have an enzyme (cytochrome b5 reductase) to convert the Hb back to the Fe$^{2+}$ state, so you are relatively healthy:

$$\text{Hb(Fe}^{3+}\text{)} + e^- \xrightarrow{\text{cytochrome b5 reductase}} \text{Hb(Fe}^{2+}\text{)}$$

People lacking functional cytochrome b5 reductase have Type I or Type II methemoglobinemia. Type I lacks the enzyme in RBC. Type II lacks the enzyme in all cells.

See:
http://www.emedicine.com/med/topic1466.htm

8. The most common type is acquired methemoglobinemia, which may result from exposure to certain types of drugs.

III. Why do chemical changes occur? (ΔG)

A. We have two goals as we try to answer this question. We want to be able to make predictions about:

1. is a compound likely to change in a given environment, and

2. if it is going to change, what products are most likely to form.

B. Concerning goal 2: A good initial way to try to make a prediction about a specific reaction is to look at patterns with structurally related chemicals. Example: Similar reactivity of halogens.

1. Cl$_2$ gas reacts vigorously with Na metal: \[ \text{Cl}_2 + 2 \text{Na} \rightarrow 2 \text{NaCl} \]

2. Can you make a prediction regarding what would happen if you mixed F$_2$ gas and Li metal? \[ \text{F}_2 + \_ \_ \text{Li} \rightarrow \_ \_ \_ \_ \_ \_ \_ \]

   Thanks, Mendeleev!!!

C. As you understand more, you can often make accurate predictions about reactions that are quite different than the ones you have previously studied.
D. Goal 1: Involves energy concerns: $\Delta G = \Delta H - T\Delta S$

1. We have been considering change as though it is an all or nothing process. It is both more accurate & useful to
not say “Will there be a reaction?”, but say “How far will the reaction go?”

2. Related to this point we have been considering all reactions to proceed only in the forward direction. Actually, at least mathematically, all reactions are at least partially reversible. That is, the forward & reverse rxns both usually occur at the same time:

\[ A + B \rightleftharpoons C + D \]

3. The $\Delta G$ in the Gibbs’ Free Energy Equation is mathematically related to “How much change will there be?”

4. Most students find that reaction coordinate diagrams improve their understanding of these issues. Let’s look at some reaction coordinate diagrams for different values of $\Delta G$:

a) The relative heights of products and reactant on the $G$ axis tell us whether the reactants will mostly change to form products or mostly stay as reactants. (Does water naturally flow uphill or downhill?)

b) The height of the hill connecting the reactant and product plateaus is related to the inherent speed (rate constant) of the rxn. (Does it take longer to walk from the 2\textsuperscript{nd} floor of the smith Building to the 4\textsuperscript{th} floor or to walk from the base to the top of Mt. Mitchell?)