

**Introduction to Hydrates**

Many ionic compounds can have water molecules incorporated into their solid structures. Such compounds are called hydrates. An ionic compound without any water locked inside its crystal structure is called an anhydrate. To emphasize the presence of discrete water molecules in the chemical structure, the formula of all hydrates shows the water of hydration separated from the rest of the chemical formula by a dot. The dot does not mean “multiply by”, it means “loosely attached to”. A coefficient before the H<sub>2</sub>O indicates the number of water molecules in the formula.

- in LAD 3.1 – Law of Constant Composition, the white substance that we heated was a hydrate. As it bubbled, water was leaving the crystal structure.
  - The name of this chemical was aluminum potassium sulfate dodecahydrate:  $KAl(SO_4)_2 \cdot 12 H_2O$
- copper(II) sulfate pentahydrate is a good example:  $CuSO_4 \cdot 5 H_2O$ 
  - (note that the number of waters is indicated by a prefix before the word hydrate)
- The formula of this deep blue compound indicates that five water molecules are associated with each CuSO<sub>4</sub> unit
  - As demonstrated in class, heating will cause the water molecules to leave the compound, and the color changes from blue to white.
- Air contains water molecules (It's called humidity.). Some anhydrous salts (those with no water trapped within their crystal structure) can absorb water directly from the air. A substance that does this is referred to as hygroscopic. In class you observed an NaOH crystal in the plastic dish as it absorbed water directly from the air. This particular salt will appear wet as it absorbs the water because it begins to dissolve as it absorbs the water. Salts that can absorb so much water from the air that they will begin to dissolve are referred to as deliquescent.

**Other examples of hydrates include:**

aluminum nitrate nonohydrate  $Al(NO_3)_3 \cdot 9 H_2O$   
 nickel(II) sulfate hexahydrate  $NiSO_4 \cdot 6 H_2O$   
 iron (III) phosphate tetrahydrate  $FePO_4 \cdot 4 H_2O$

Unfortunately, the number of water molecules that get locked inside the crystal structure cannot be determined by looking at the chemical formula unit. The number of water molecules, which can range from 0 to as high as 18, must be determined by doing experiments. In fact some ionic compounds exist in several different forms with different numbers of water molecules.

**Theoretical % composition of a hydrate (% of water in a hydrate)**

Mass percentages might also be used to analyze a hydrate such as copper(II) sulfate pentahydrate

Using theoretical values:

for the compound:  $CuSO_4 \cdot 5 H_2O$

$$CuSO_4 \quad 63.54 \text{ g/mole} + 32.07 \text{ g/mole} + 4(16.0 \text{ g/mole}) = 159.61 \text{ g/mole}$$

$$H_2O \quad 5 [ 2(1.01 \text{ g/mole}) + 16.0 \text{ g/mole} = 18.02 \text{ g/mole} ] = 90.1 \text{ g/mole} \quad 249.71 \text{ g/mole total}$$

therefore the theoretical percentage of water in the copper sulfate hydrate can be calculated

$$\frac{90.1}{249.71} = 0.360 \quad \text{which is } 36.0 \%$$

**Experimental % composition of a hydrate (% of water in a hydrate)**

Mass percentages might also be used to analyze a hydrate such as copper(II) sulfate pentahydrate

Using experimental values: (as demonstrated in class)

mass of hydrate (g)	2.75
mass of anhydrate (g)	1.90

from these two numbers you can subtract to determine the mass of water that was heated away.

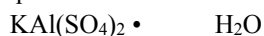
$$2.75 \text{ g} - 1.90 \text{ g} = 0.85 \text{ g of water}$$

$$\frac{0.85}{2.75} = 0.309 \quad \text{which is } 30.9 \%$$

## Empirical formulas for the water in hydrate salts

Let's say you didn't know how many water molecules were attached to some hydrated salt. You could calculate it from data gathered by heating the salt and turning it into an anhydrate as in LAD 3.1A – The Mass Ratio of SG

As discussed in class, SG was actually the compound potassium aluminum sulfate hydrate whose formula is



and we would like to determine the formula of the hydrate given the data below.

mass of hydrate (g)	1.755
mass of anhydrate (g)	0.956

To determine the formula of this hydrate, you must determine the mole ratio of salt to water so you can fill in the blank in the formula of the hydrate shown above. The steps are strikingly similar to the same steps that you used to determine empirical formulas of ionic compounds.

- First you must realize that from these two data you can subtract to determine the mass of water that was heated away.
  - $1.755 - 0.956 \text{ g} = 0.799 \text{ g}$
- next, convert both mass values to moles
  - water  $0.799 \text{ g} \left( \frac{1 \text{ mol}}{18 \text{ g}} \right) = 0.0444 \text{ mole of water}$
  - “dry” salt  $0.956 \text{ g} \left( \frac{1 \text{ mol}}{258.3 \text{ g}} \right) = 0.00370 \text{ mole of anhydrate (be careful to NOT round off too much)}$
- then, divide by the smaller mole value.
  - water  $\frac{0.0444}{0.00370} = 12$
  - “dry” salt (anhydrate)  $\frac{0.00370}{0.00370} = 1$
- Voilà
  - The formula must be  $\text{KAl}(\text{SO}_4)_2 \cdot 12 \text{ H}_2\text{O}$
  - We would name this compound: potassium aluminum sulfate dodecahydrate

### If the problem were reported in percentages, the procedure is nearly the same:

For the salt potassium aluminum sulfate hydrate;  $\text{KAl}(\text{SO}_4)_2 \cdot \text{ \_\_\_\_ } \text{H}_2\text{O}$ , if percentage of water in the hydrate was analyzed to be 45.5 %, determine the formula of the hydrate.

- First you should realize that from this water percentage you can subtract to determine “dry” salt percentage.
  - $100\% - 45.5\% = 54.5\%$
- next, convert both mass values to moles
  - water  $45.5\%(g) \left( \frac{1 \text{ mol}}{18 \text{ g}} \right) = 2.53 \text{ mol}$
  - “dry” salt  $54.5\%(g) \left( \frac{1 \text{ mol}}{258.3 \text{ g}} \right) = 0.211 \text{ mole (be careful to NOT round off too much)}$
- then, divide by the smaller mole value.
  - water  $\frac{2.53}{0.211} = 11.99$
  - “dry” salt  $\frac{0.211}{0.211} = 1$
- and, Voilà
  - (as before) the formula must be  $\text{KAl}(\text{SO}_4)_2 \cdot 12 \text{ H}_2\text{O}$

*one more problem type on the next page*

**If the problem did not tell you the formula of the anhydrate, you must first determine its empirical formula and then proceed on to determining the anhydrate to water mole ratio:**

Some hydrate was 43.7 % water. The polyatomic ion portion of the compound was made of 34.5% iron and 65.6% chlorine. Determine the chemical formula of this hydrate, then name it.

In this problem it is very important to realize that this is a *two part* problem – you must first determine the empirical formula of the anhydrate ionic compound. Then you can proceed on to determining the moles of water in the hydrated salt.

- First, the empirical formula of the iron chloride anhydrate. Convert percentages (used as mass values) to moles.

$$\circ \text{ Fe } 34.4\%(g) \left( \frac{1\text{mol}}{55.85\text{g}} \right) = 0.616 \text{ mole}$$

$$\circ \text{ Cl } 65.6\%(g) \left( \frac{1\text{mol}}{35.45\text{g}} \right) = 1.85 \text{ moles}$$

- Proceed to step 2.

$$\circ \text{ Fe } \frac{0.616}{0.616} = 1$$

$$\circ \text{ Cl } \frac{1.85}{0.616} = 3.0$$

- Voilà

- The empirical formula of the anhydrate must be  $\text{FeCl}_3$

Next you must compute the mole ratio between the water and the “dry” salt.

- First you should realize that from this water percentage you can subtract to determine “dry” salt percentage.

$$\circ 100\% - 43.7\% = 56.3\%$$

- next, convert both mass values to moles

$$\circ \text{ water } 43.7\%(g) \left( \frac{1\text{mol}}{18\text{g}} \right) = 2.43 \text{ mole}$$

$$\circ \text{ “dry” salt } 56.3\%(g) \left( \frac{1\text{mol}}{162.35\text{g}} \right) = 0.347 \text{ mole (be careful to NOT round off too much)}$$

- Proceed to step 2 (skip 3)

$$\circ \text{ water } \frac{2.53}{0.347} = 7$$

$$\circ \text{ “dry” salt } \frac{0.347}{0.347} = 1$$

- and, Voilà

- the formula must be  $\text{FeCl}_3 \cdot 7 \text{H}_2\text{O}$  iron(III) chloride heptahydrate