

C125 Experiment #9
Prep and Analysis of a Coordination Compound
Calculations

Use the following example calculations to assist you with calculating the theoretical % yield, the experimental % yield, and the % purity of the potassium trioxalato ferrate (III) trihydrate crystals synthesized. These examples correspond to the “Calculations” section on page 4, Exp #9 of the lab manual.

- When typing chemical formulas and equations in “Word”, click on the “Format” button on the menu line, scroll down to “Font” and use subscript and superscript as required. Two dashes and a greater than sign make an arrow: \rightarrow . Once a formula has been typed, use the “Edit” button to copy and paste where you need formulas in other places.
- Calculate the % oxalate ($\text{C}_2\text{O}_4^{2-}$) in pure $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]\cdot 3\text{H}_2\text{O}$.

EXAMPLE: Calculate the % permanganate in potassium permanganate.

$$\begin{aligned} & \% \text{MnO}_4^- \text{ in } \text{KMnO}_4 \\ & (\text{fw } \text{MnO}_4^- = 118.94 \text{ g/mol}; \text{ fw } \text{KMnO}_4 = 158.04 \text{ g/mol}) \\ & \% \text{MnO}_4^- = \frac{118.94 \text{ g/mol}}{158.04 \text{ g/mol}} \times 100 \% = 75.26 \% \end{aligned}$$

- Calculate the theoretical yield of trioxalato ferrate (III) trihydrate (green crystals).

EXAMPLE: If the starting mass of ferrous ammonium sulfate was 5.000 g, what is the theoretical yield of green crystals, potassium trioxalato ferrate (III) trihydrate?

- The following abbreviations have been used:
 sm = starting material = $(\text{NH}_4)_2[\text{Fe}(\text{H}_2\text{O})_2(\text{SO}_4)_2]\cdot 4\text{H}_2\text{O}$
 yp = yellow precipitate = $\text{Fe C}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$
 gc = green crystals = $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]\cdot 3\text{H}_2\text{O}$

$$5.000 \text{ g sm} \times \frac{1 \text{ mol}}{392.14 \text{ g}} \times \frac{1 \text{ mol yp}}{1 \text{ mol sm}} \times \frac{2 \text{ mol gc}}{2 \text{ mol yp}} \times \frac{491.26 \text{ g}}{1 \text{ mol gc}} = 6.2638 \text{ g green crystals}$$

- Calculate the experimental PERCENT yield. Note: The experimental % yield is always less than the theoretical yield. The experimental % yield is always $< 100\%$.

EXAMPLE: If the amount of green crystals collected in the laboratory was 5.9801 g, what is the experimental % yield?

$$\% \text{ yield} = \frac{\text{experimental yield}}{\text{theoretical yield}} \times 100 = \frac{5.9801 \text{ g}}{6.2638} \times 100 = 95.470 \%$$

5. Preliminary titration calculation: Calculate the amount of green crystal sample to use for a titration so that the volume of titrant (potassium permanganate) is within that contained in the buret (< 50 mL).

EXAMPLE: Calculate the mass of green crystals to use in order that the volume of potassium permanganate needed to reach the endpoint of the titration is about 20 mL.

$$\text{Let } [\text{KMnO}_4] = 0.0200 \text{ M} = 0.0200 \text{ mol KMnO}_4 / \text{L}$$

Think: You will be using potassium permanganate to react with the oxalate ion according to the equation given on page 2, Exp #9. By definition, the endpoint is reached when the reactants have been consumed in equivalent stoichiometric amounts.

Here are the steps: Use 0.0200 M KMnO_4 to react with the oxalate ion in a sample of trioxalato ferrate (III) trihydrate crystals (green crystals, gc). The maximum volume of KMnO_4 which a buret can hold is 50 mL. Therefore, try to use about half that volume of titrant (~ 20 mL).

STEPS: concentration titrant x volume desired x the stoichiometric relationships from the balanced equations and formulas for the titrant to totally react with the sample x conversion from moles to grams of sample

$$\frac{0.0200 \text{ mol KMnO}_4}{1 \text{ L}} \times 0.020 \text{ L} \times \frac{1 \text{ mol MnO}_4^-}{1 \text{ mol KMnO}_4} \times \frac{5 \text{ mol C}_2\text{O}_4^{2-}}{2 \text{ mol MnO}_4^-} \times \frac{1 \text{ mol gc}}{3 \text{ mol C}_2\text{O}_4^{2-}} \times \frac{491.27 \text{ g}}{1 \text{ mol gc}}$$

$$= 0.164 \text{ g green crystals}$$

*About 0.16 g trioxalato ferrate (III) trihydrate should be massed to be use in each of the three titrations to be performed.

6. Calculate the % oxalate in synthesized green crystals.

EXAMPLE: Given the following data collected from titration:

Mass green crystals Trial #1 = 0.1873 g, $[\text{KMnO}_4] = 0.0207 \text{ M}$, Titration volume = 19.30 mL KMnO_4

- a. Calculate g $\text{C}_2\text{O}_4^{2-}$ in product: (mol KMnO_4 to mol MnO_4^- to mol $\text{C}_2\text{O}_4^{2-}$ to g $\text{C}_2\text{O}_4^{2-}$)

$$\frac{0.0207 \text{ mol KMnO}_4}{1 \text{ L}} \times 0.01930 \text{ L} \times \frac{1 \text{ mol MnO}_4^-}{1 \text{ mol KMnO}_4} \times \frac{5 \text{ mol C}_2\text{O}_4^{2-}}{2 \text{ mol MnO}_4^-} \times \frac{88.022 \text{ g}}{1 \text{ mol C}_2\text{O}_4^{2-}} = 0.08791 \text{ g}$$

- b. Calculate % oxalate.

$$\frac{\text{g oxalate in green crystals}}{\text{g green crystals in sample}} \times 100\%$$

$$\% \text{ oxalate} = \frac{0.08791 \text{ g}}{0.1873 \text{ g}} \times 100 = 46.94 \% \text{ oxalate}$$

9. Calculate the % purity of the crystals. Theoretical % oxalate (calc #2) = 53.75 %

Method 1: % purity = $\frac{\text{experimental \% oxalate}}{\text{theoretical \% oxalate}} \times 100\%$

$$\% \text{ purity} = \frac{46.94 \%}{53.75 \%} \times 100 = 87.33 \%$$

Method 2:

$$\% \text{ purity} = \frac{\text{g oxalate from titration}}{\text{theoretical g oxalate from crystals}} \times 100\%$$

EXAMPLE:

1. Calculate the theoretical g oxalate in the sample, 0.1873 g.

$$0.1873 \text{ g gc} \times \frac{1 \text{ mol}}{491.27 \text{ g gc}} \times \frac{3 \text{ mol } C_2O_4^{2-}}{1 \text{ mol } K_3[Fe(C_2O_4)_3] \cdot 3H_2O} \times \frac{88.022 \text{ g}}{1 \text{ mol } C_2O_4^{2-}} = 0.1007 \text{ g}$$

2. Find the % purity.

$$\% \text{ purity} = \frac{\text{g oxalate recovered}}{\text{theoretical g oxalate}} \times 100 = \frac{0.08791 \text{ g}}{0.1007 \text{ g}} \times 100 = 87.30 \%$$