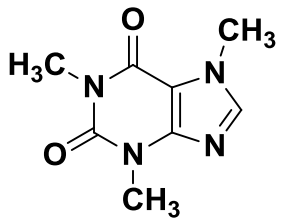
PW 4: Extraction of an Organic Compound (Extraction of Caffeine from COCA-COLA

1. Objectives

Model the mechanism of caffeine extraction using an organic solvent by drawing behavioral analogies between the chemical species involved.

2. Caffeine

Caffeine (**1,3,7-trimethylxanthine**) **$C_8H_{10}N_4O_2$**. Pure caffeine is dangerous because it has a significant effect on the body: insomnia, heart palpitations, nausea, anxiety, and polyuria. The estimated lethal dose (average fatal quantity) is between 5 and 10 grams for an adult. **Do not taste pure caffeine!** When taken in high doses, coffee (and caffeine) can be considered a drug.



caffeine

3. Materials and Chemicals

Materials	Chemicals
-Separatory funnel - Condenser - Round-bottom flask - Heating magnetic stirrer - - Magnetic stirring bar - - Büchner funnel - 100 mL Erlenmeyer flask - pH paper	- 100 mL of COCA COLA. - Calcium carbonate ($CaCO_3$) - Anhydrous magnesium sulfate or sodium sulfate, or alternatively anhydrous calcium chloride - Dichloromethane or chloroform - Water

4. Procedure

- Measure 100 mL of Coca-Cola into an Erlenmeyer flask.
- Add dropwise a sodium carbonate solution, while monitoring the pH.
- Stop the addition when the pH reaches 9.
- Pour the mixture into a 250 mL beaker and then add 100 mL of dichloromethane.
- Stir under a fume hood using a magnetic stirrer.
- Then extract the phase containing the caffeine using a separatory funnel.
- Shake the mixture (don't forget to release the pressure from time to time).
- Let it settle (allow it to rest for **30 seconds**).
- Collect the organic phase (colored dichloromethane – it's the bottom layer!).
- Combine the two organic phases (colored solutions).
- It is advisable to keep the aqueous phases until the end of the experiment, just in case!
- Dry the organic phase using calcium carbonate. There is no defined amount to add. You should add it until there are no more clumps. Don't be afraid to add more it's not dangerous. It's better to add too much than too little.
- Filter everything using a funnel containing a piece of cotton.
- Collect the filtrate and evaporate the solvent using a rotary evaporator.
- You will be left with a powder at the bottom of your flask—that's nearly pure caffeine.

Questions

- What is the purpose of the reflux setup? Why is heating necessary? What is the role of the condenser?
- What is the role of the boiling stones?
- Calculate the yield of the extraction.
- Is caffeine a natural or artificial substance?
- What is the difference between **caffeine** and **theine**?
- What is the purpose of adding anhydrous magnesium sulfate?
- What is the purpose of adding calcium carbonate?