Conceptual Chemistry

Introduction to Molecular Spectroscopy: Glow In The Dark Explorations with Tonic Water and Colorimetric Analysis of Tabletop Sweeteners

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Conceptual Chemistry

Conceptual Chemistry is a graduate course designed for grade school and middle school teachers to assist in their understanding of chemistry and to provide concrete ideas that they can take back to their classrooms to teach their students.

Conceptual Chemistry

Participants in this course receive:

- Free tuition and five graduate credit hours from the College of Education of Kent State University. *($2,340 value)*
- Over $850 worth of materials and supplies to take back to the classroom.

Conceptual Chemistry

Support for *Conceptual Chemistry* and the development/production of this material was provided by a grant under the federally funded *Improving Teacher Quality State Grants Program*, administered by the Ohio Board of Regents.

Spectroscopy

Spectroscopy
The investigation into the nature of matter using electromagnetic radiation.

Most Common Types
Infrared, ultraviolet, visible, NMR, X-ray and microwave.

Activity Objectives

Key concepts:

- Molecular Spectroscopy
- Chemical Changes
- Physical Changes
- Quantitative and Qualitative Analyses
- Having fun with science!

Spectroscopic Analysis

Purpose

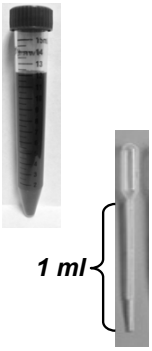
To determine the concentration of drink mix in an unknown sample using semi-quantitative visible light spectroscopy.

Spectroscopic Analysis

Materials

12 ml Raspberry Crystal Light
distilled water
6 glass test tubes
1.0 ml graduate plastic pipet
visible light source

Crystal Light is diluted per instructions: 1 pkg. in 500 ml water.



Spectroscopic Analysis

Procedure

1. Obtain a 15 ml plastic conical tube containing Crystal Light drink mix *(12 ml "stock" solution).*
2. Use a plastic pipette to withdraw 8.0 ml of Crystal Light drink mix from the conical tube containing the "stock" solution and place it into the *first* test tube. *(This leaves 4.0 ml drink mix in the plastic tube.)*

Spectroscopic Analysis

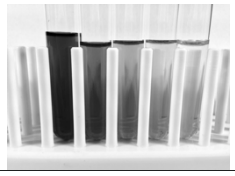
Procedure (cont.)

3. Add 8.0 ml water to the plastic conical tube, replace the cap and mix thoroughly. *(This gives 12 ml of solution again!)*
4. Withdraw 8.0 ml of the diluted Crystal Light drink mix from the conical tube and place it into the *second* test tube. *(This leaves 4.0 ml drink mix in the plastic tube again.)*

Spectroscopic Analysis

Procedure (cont.)

5. Add 8.0 ml water to the plastic conical tube, replace the cap and mix thoroughly.
6. Continue this dilution process three more times until *five* glass test tubes are filled.

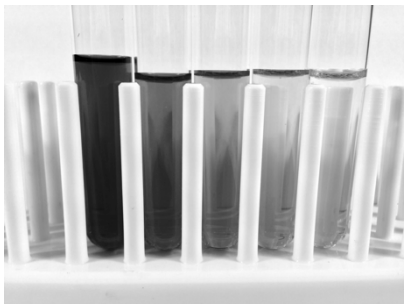


Spectroscopic Analysis

Procedure (cont.)

7. Obtain a conical tube containing the *"unknown"* sample. Place 8.0 ml of the *"unknown"* into the *sixth* test tube.
8. Compare the *"unknown"* sample to the five standards to determine the dilution ratio of the unknown sample. (1.9 g drink mix dissolved into 500 ml water).

Spectroscopic Analysis



Spectroscopic Analysis

Dilution Math

$$3.8\ g/L \times \frac{4\ ml}{12\ ml} = 1.3\ g/L$$

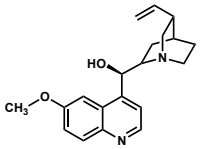
Tube #1	Tube #2	Tube #3	Tube #4	Tube #5
3.8 g/L	1.3 g/L	0.43 g/L	0.14 g/L	0.058 g/L

"Unknown" was prepared to match "Tube #2"

Spectroscopic Analysis

Purpose

To determine the concentration of *quinine* in tonic water using qualitative spectroscopy.



quinine

Spectroscopic Analysis

Materials

12 ml tonic water
Distilled water
6 glass test tubes
1.0 ml graduate plastic pipet
UV light source

Tonic water is used as purchased and assumed to contain 60 mg/L quinine

Spectroscopic Analysis

Procedure

1. Obtain a 15 ml plastic conical tube containing tonic water *(12 ml "stock" solution).*
2. Use a plastic pipette to withdraw 8.0 ml of tonic water from the conical tube containing the "stock" solution and place it into the *first* test tube. *(This leaves 4.0 ml tonic water solution in the plastic tube.)*

Spectroscopic Analysis

Procedure (cont.)

3. Add 8.0 ml water to the plastic conical tube, replace the cap and mix thoroughly. *(This gives 12 ml of solution again!)*
4. Withdraw 8.0 ml of the diluted tonic water from the conical tube and place it into the *second* test tube. *(This leaves 4.0 ml drink mix in the plastic tube again.)*

Spectroscopic Analysis

Procedure (cont.)

5. Add 8.0 ml water to the plastic conical tube, replace the cap and mix thoroughly.
6. Continue this dilution process three more times until *five* glass test tubes are filled.
7. Shine a UV light onto the test tubes being careful not to expose yourself or others to the light. Note the variable brightness of the tubes with respect to concentration.

Spectroscopic Analysis

Procedure (cont.)

8. Obtain a conical tube containing the *"unknown"* sample. Place 8.0 ml of the *"unknown"* into the *sixth* test tube.
9. Compare the "unknown" sample to the five standards to determine the dilution ratio of the unknown sample. (60 ppm quinine is dissolved into 1,000 ml solution).

Spectroscopic Analysis

Dilution Math

Tonic water is regulated and may only contain up to 83 ppm of quinine. Most commercial tonic water ranges from 25 -60 ppm.

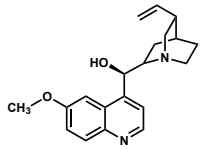
$$60 \text{ ppm} \times \frac{4 \text{ ml}}{12 \text{ ml}} = 20 \text{ ppm}$$

Tube #1	Tube #2	Tube #3	Tube #4	Tube #5
60 ppm	20 ppm	6.7 ppm	2.2 ppm	0.70 ppm

"Unknown" was prepared to match "Tube #3"

History of Tonic Water

Quinine is an anti-pyretic, anti-inflammatory, analgesic, anti-malarial bitter tasting drug and has been used for hundreds of years to treat malaria symptoms.



Ultraviolet Light

UV-A

320-400 nm, lowest energy UV light, suspected of damaging skin (premature aging and wrinkling), and skin cancer.

UV-B

280-320 nm, affects DNA, eyes, immune system. UV radiation at 280 nm is 10^5 times more damaging than UV radiation at 320 nm.

UV-C

10 - 280 nm, (10 nm – 120 nm is *ionizing* EMR) very high energy, most harmful.

Ultraviolet Light

UV-A

320-400 nm, lowest energy UV light, suspected of damaging skin (premature aging and wrinkling), and skin cancer.

Modified Biuret Reagent

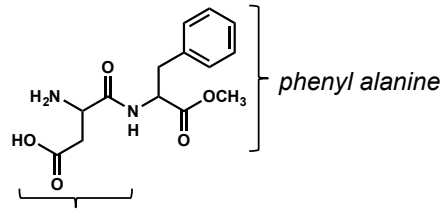
Modified Biuret Reagent

Biuret Reagent (250 mL): Copper (II) sulfate pentahydrate (3.75 g, 15.0 mmol) was added to a 250 mL volumetric flask. Water was added (40 mL) and the copper (II) sulfate pentahydrate was completely dissolved. A solution of potassium sodium tartrate tetrahydrate (18.82 g, 52.5 mmol) in water (60 mL) was prepared in a separate container and combined with the copper (II) sulfate solution. Finally, dilute the mixture to volume using 1 M sodium carbonate solution.

Modified Biuret Reagent

Sodium Carbonate (1 M): Sodium carbonate (105.99 g, 1 mol) was added to a 1 L volumetric flask and dissolved into 750 mL water. The solution was then diluted to volume with water.

NutraSweet®



phenyl alanine

aspartic acid

methyl ester of a dipeptide

Qualitative Analysis

1. Use dropper bottle to add 20 drops of reference materials to 24 well plate.

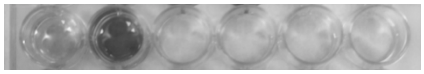
Addition Order

B1: water, B2: aspartame solution

2. Add 5 drops biuret reagent.

3. Note results.

Qualitative Analysis



Qualitative Analysis

1. Label plastic conical tubes (5):

   Equal®, sugar, Splenda®, Sweet One®, Sweet 'N Low®

2. Add 1 pkg. sweetener to 15 ml plastic conical tube.
3. Fill to volume (14 ml) with water, cap and mix.

Qualitative Analysis

1. Use a plastic pipet to add 1 ml of sweetener sample solution to 24 well plate.

Addition Order

C1: Equal®, C2: sugar, C3: Spenda®

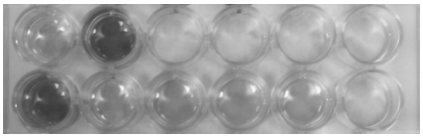
C4: Sweet One®, C5: Sweet 'N Low®

2. Add 5 drops biuret reagent.
3. Note results.

1 ml

Qualitative Analysis

aspartame



NutraSweet contains aspartame!

Tabletop Sweeteners

Sugar – sucrose (dextrose & fructose)

Equal® – aspartame, dextrose & maltodextrose (maltodextrin)

Sweet 'N Low® – saccharine, dextrose and maltodextrose (maltodextrin)

Sweet One® – acesulfame-K, dextrose, cream of tartar, calcium silicate

Splenda® – sucralose, dextrose and maltodextrin

Dextrose, Sucrose and Maltodextrin

1 g carbohydrate = 4 calories

sucrose, glucose and maltodextrin are carbohydrates!

No cal sweeteners contain 4 calories but they meet the FDA label requirement for a zero calorie supplement!

Spectroscopic Analysis

- According to the Beer-Lambert Law, concentration of a solution is directly proportional to its absorption of electromagnetic radiation.

$$A = \varepsilon bc$$

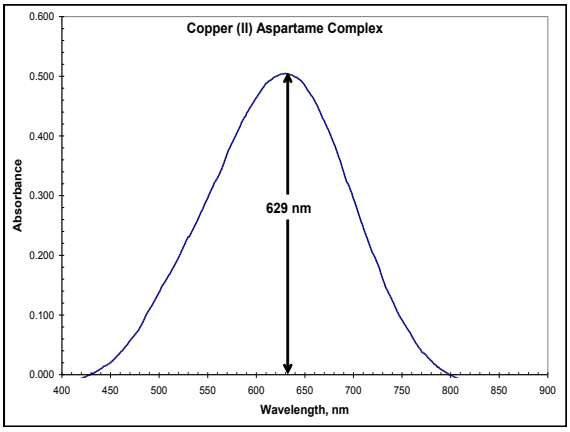
Where:

A = absorbance

ε = molar absorptivity coefficient

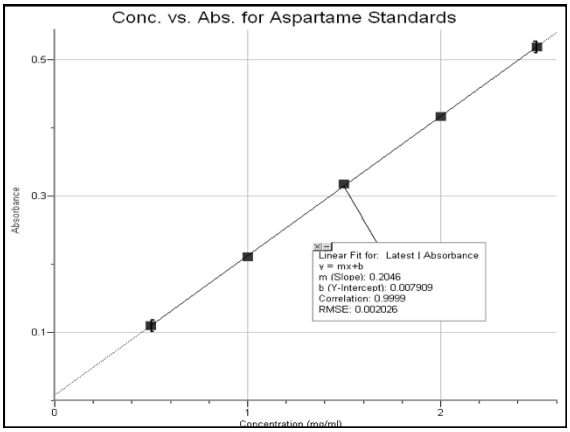
b = sample cell path length

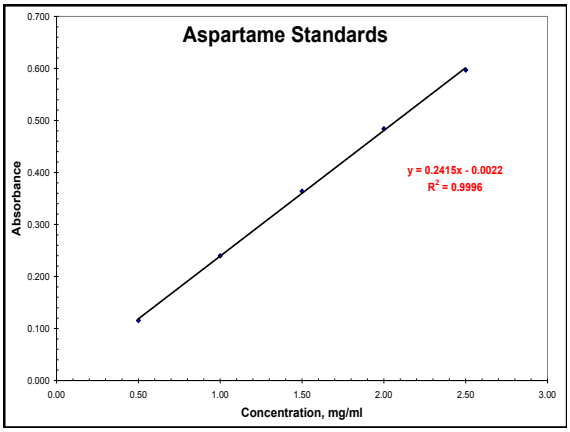
c = sample concentration



Method

1. Prepare a stock aspartame solution (5.00 mg/ml).
2. Prepare reference standards; 0.50 mg/ml, 1.00 mg/ml, 1.50 mg/ml, 2.00 mg/ml and 2.50 mg/ml by reaction of standard with 2.00 ml biuret reagent and dilution.
3. Wait 15 minutes and collect spectroscopic data at 629 nm.
4. Prepare and analyze Equal® samples





Spectroscopic Analysis

For 14 trials:

$y = 0.2415x - 0.0022$

$r^2 = 0.9996$

For 44 Equal® Samples:

aspartame per sample = 37.6 ± 2 mg/g

manufacturer's claim = 38 mg/g

1.05% difference!

Conclusions

- New method for identifying and determining the amount of aspartame in tabletop sweeteners.
- Analysis of 44 samples gave 37.6 mg ± 2 mg aspartame/g Equal® observed compared to 38 mg/g as stated by the manufacturer. (1.05% difference)

- Christopher J. Fenk, Donald G. Gerbig, Jr. and Nathan Kaufman "A New Colorimetric Assay of Tabletop Sweeteners Using a Modified Biuret Reagent" *J. Chem. Educ.* **2007**, *84* (*10*), 1676-1678.

Conclusions

- Methods for introducing the concepts of spectroscopic analysis of samples were presented.
- Both visible and UV light were used to semi-quantitatively determine the concentration of unknown samples.
- Unknowns are determined using the oldest/ most sophisticated detection device known. Your eyes.