

COLOUR CHEMISTRY

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PURPOSE OF EXPERIMENT

The purpose of the experiment was to investigate the emission spectra of a series of unknown metal salt solutions upon heating and identify its component elements. The emission of light from metal cations upon heating is extremely useful in the field of pyrotechnic chemistry; it is used for illumination and signalling in a variety of manners and the colour of the emission can be tailored by the use of a variety of compounds. This theory has also been used to develop pyrotechnic compounds that can emit IR wavelengths to be used as decoys countermeasures for IR seeking missiles [1]. Each element will have a unique emission spectra which is utilised in astronomy and chemistry to categorise what has been observed into its component elements. This experiment was done by eye which is subjective however optical spectrographs have been developed to provide discrete data of the observed emissions.



FIGURE 1 - COLOUR CHEMISTRY IN USE IN CIVIL AND MILITARY SETTINGS [2]

THEORY

Atoms contain their electrons in ladder-like quantized energy levels or shells [3] as shown in Figure 2. These shells also contain subshells (S, P, D, F). Electrons in the outermost shells from the nuclei are referred to as valence electrons, the quantity of which corresponds to group of the element. These electrons can be 'excited' by external energy and temporarily jump to a higher shell. These 'jumps' can be considered as rungs on a ladder, the electron cannot exist between the rungs and each 'ladder' is unique to the element; therefore these energy levels can be quantized and discrete elements can be identified by these energy levels. This elevation in energy level is temporary as systems naturally want to return to a more stable lower energy level, the electrons ground state [4]. To reach the ground state the electron must release this additional energy in the form of a photon of a frequency that corresponds to the emitted energy $e = h \times f$ where h is Planck's constant: 6.6262×10^{-34} [5]. From this equation you can calculate the wavelength of this photon with the equation: $\lambda = \frac{c}{f}$ where c is the speed of light ($299,792,458 \text{ ms}^{-1}$, often simplified to $3 \times 10^8 \text{ ms}^{-1}$ [6]).

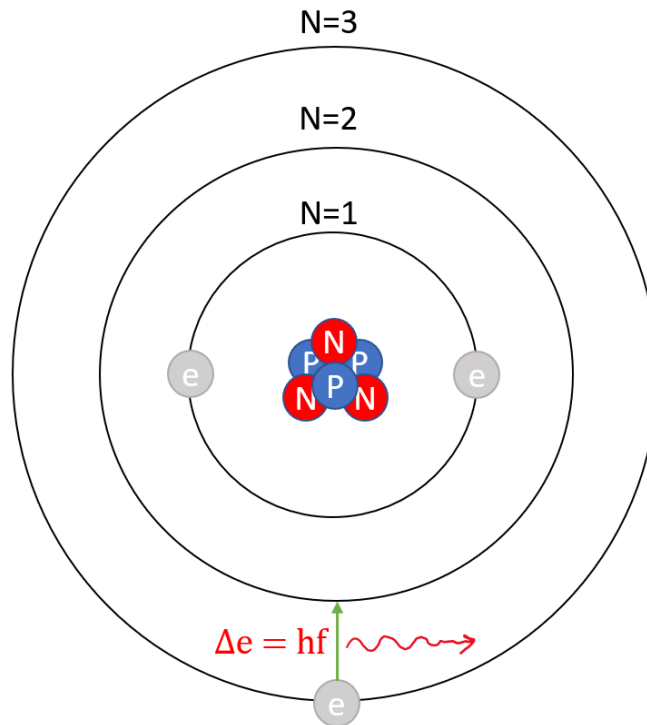


FIGURE 2 - BOHR'S MODEL LITHIUM ATOM WITH AN EXCITED VALENCE ELECTRON EMITTING A PHOTON (RED ARROW)

As seen in the energy calculations later; Joules are too large to be used on an atomic scale as the results are in the 10^{-19} scale. Therefore the unit electronVolt is used with a conversion factor of $1\text{J}=6.25\times10^{18}\text{eV}$; this is calculated from accelerating an electron of charge e through a potential difference of 1V [7]. Visible light exists within a middle ground where their photons have enough energy due to their frequency to display the properties of discrete particles; but their wavelength is sufficiently long for properties of waves to be observed.

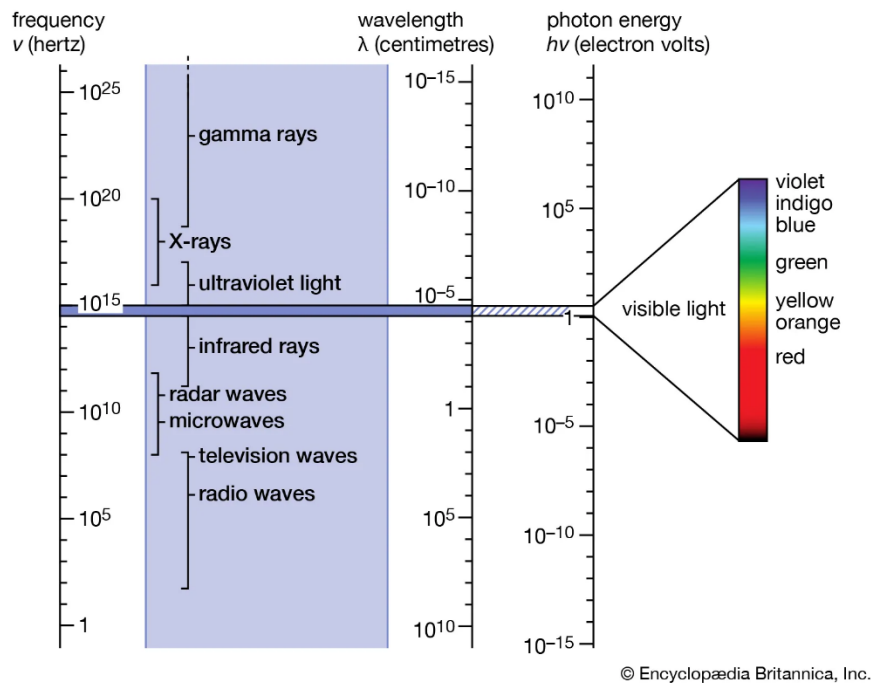


FIGURE 3 - THE ELECTROMAGNETIC SPECTRUM [8]

In this experiment the emission spectra were observed by the operators eyes. This introduces subjectivity which is inappropriate for scientific applications, however it is adequate for the demonstration of the theory. To obtain quality data, optic optical spectrometers are utilised this is able to measure the incoming wavelength of the light and output this data.

APPLICATIONS IN OME & BEYOND

Pyrotechnics use a variety of metal salt compounds within flares, decoys and smoke grenades for a tailored colour effect. Some colour agents can also be used as oxidizers, such as barium chlorate; to increase the burning properties of the composition at the same time as providing visual output. The most obvious use of this colour chemistry seen in our day-to-day lives is within fireworks. For example, strontium produces a deep red and copper produces blue light. The reverse of this application is observing our universe, astronomers can use spectrometry to analyse planets and stars to quantify what elements they are composed of.

PROCEDURE

CHEMICALS AND HAZARDS

Chemical hazard information for the 1M salt solutions was from the taken the provided worksheet, Appendix B. These hazards are mitigated by the use of correct PPE and the appropriate laboratory awareness. The PPE required for the experiment was a fastened lab coat, safety goggles and disposable gloves. A briefing laid out the roles and responsibilities of the students and the procedure for accidents; the laboratory manager was to be notified immediately so that they could safely dispose of the solutions.

The salt solutions are named as such due to their ionic bonding. The metal loses its valence electrons to become a positively charged cation and reacts a chlorine atom which has gained an electron, becoming an anion. The anion is denoted by the suffix 'ide'. For example, consider Copper Chloride (CuCl_2) depicted in Figure 3.

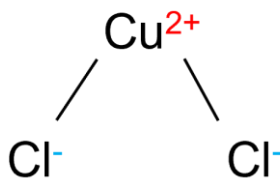


FIGURE 2 - DIAGRAM OF CuCl_2 TO ILLUSTRATE CATION AND ANION

EQUIPMENT

- Heat-resistant mat
- Bunsen burner
- Matches
- Nichrome wire loop
- Blue cobalt glass
- Beaker containing deionized (DI) water
- Beakers containing 1M unknown salt solutions labelled A-H

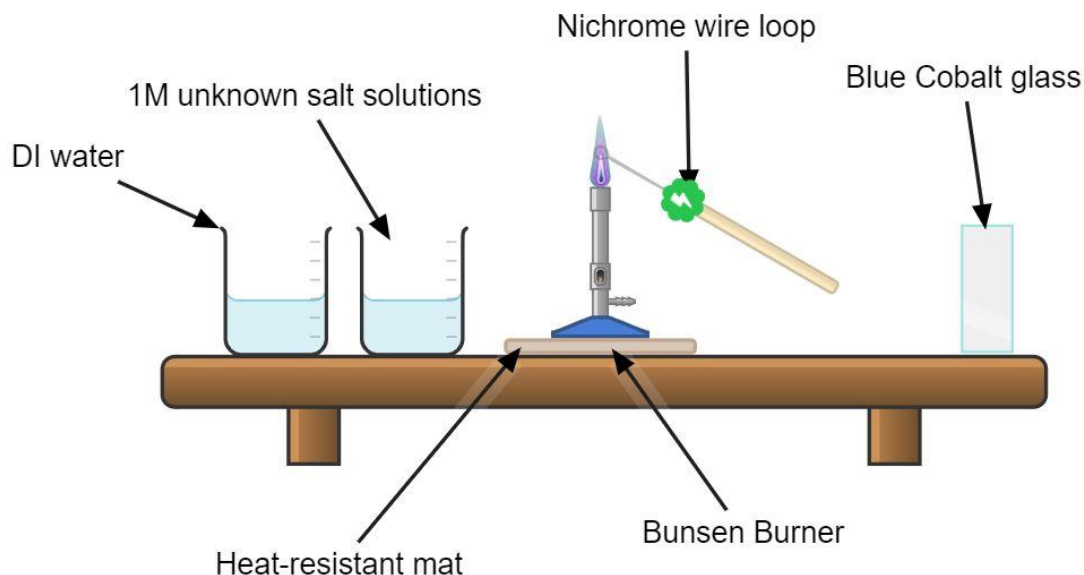


FIGURE 3 - PRACTICAL EQUIPMENT SETUP

METHOD

1. Set up the Bunsen burner on the heat-resistant mat and layout the equipment with reference to figure 4
2. Ensure the Bunsen burner air vent is closed and light it. A yellow flame will be emitted, this is the 'safety flame' and should be used when the salt solutions are not directly being tested.
 - a. For testing of the solutions a hotter, fuel-lean oxygen rich flame is required. This is achieved by opening the air vent resulting in inner flame cone in which the sample under test should be located.
3. Dip the wire loop into the DI water and heat in the inner flame cone.
 - a. Allow the wire loop to cool
4. Dip the wire into the unknown salt solution and heat in the inner flame cone
5. Observe the flame colour visually and then repeat step 4, observing the flame colour through the blue Cobalt glass.
6. Write down the result in the provided worksheet and repeat the cleaning step 3 before moving onto the next salt solution with step 4.

RESULTS

Unknown Metal Salt	Flame Colour	Flame Colour (through Cobalt glass)	Identified Metal	Wavelength [nm]
(De-Ionised Water)	Orange	Orange	NA	600
A	Red/Pink	Yellow	Inconclusive	700
B	Red	Red	Strontium	650
C	Orange	Orange	Calcium	600
D	Violet	Violet	Barium	400
E	Yellow	Yellow	Sodium	580
F	Ruby Red	Yellow	Lithium	700
G	Green/Blue	Green	Copper	500-550
H	Orange	Lavender	Potassium & Sodium	600 (Na) / 400-450 (K)

TABLE 1 - RESULTS FROM EXPERIMENT (APPENDIX A) WITH WAVELENGTHS MATCHED FROM LITERATURE [9]

ENERGY CALCULATIONS

Flame Colour	Flame Colour (through Cobalt glass)	Identified Metal	Wavelength [nm]	Frequency [Hz]	Energy [J]	Energy [eV]
Orange	Orange	NA	600	4.99654×10^{14}	3.31081×10^{-19}	2.067
Red/Pink	Yellow	Inconclusive	700	4.28275×10^{14}	2.83784×10^{-19}	1.771
Red	Red	Strontium	650	4.61219×10^{14}	3.05613×10^{-19}	1.908
Orange	Orange	Calcium	600	4.99654×10^{14}	3.31081×10^{-19}	2.067
Violet	Violet	Barium	400	7.49481×10^{14}	4.96621×10^{-19}	3.100
Yellow	Yellow	Sodium	580	5.16884×10^{14}	3.42497×10^{-19}	2.138
Ruby Red	Yellow	Lithium	700	4.28275×10^{14}	2.83784×10^{-19}	1.771
Green/Blue	Green	Copper	525	5.71033×10^{14}	3.78378×10^{-19}	2.362
Orange	Lavender	Potassium	760	3.94464×10^{14}	2.6138×10^{-19}	1.632
		Sodium	589	5.08985×10^{14}	3.37264×10^{-19}	2.105

TABLE 2 – PHOTON ENERGY CALCULATIONS FROM OBSERVED FLAME COLOURS

Metal ion	Flame Colour	Wavelength [nm]	Frequency [Hz]	Energy [J]	Energy [eV]
Ba^{2+}	Green/Yellow	577	5.19571×10^{14}	3.44278×10^{-19}	2.149
Ca^{2+}	Orange	609	4.9227×10^{14}	3.26188×10^{-19}	2.036
Li^+	Red/Pink	670	4.47451×10^{14}	2.9649×10^{-19}	1.851
Sr^{2+}	Red	650	4.61219×10^{14}	3.05613×10^{-19}	1.908
K^+	Lavender	760	3.94464×10^{14}	2.6138×10^{-19}	1.632
Na^+	Yellow	589	5.08985×10^{14}	3.37264×10^{-19}	2.105
Cu^{2+}	Blue/Green	525	5.71033×10^{14}	3.78378×10^{-19}	2.362

TABLE 3 - PHOTON ENERGY CALCULATIONS (FLAME COLOURS AND WAVELENGTHS TAKEN FROM LITERATURE [10] [11])

DISCUSSION

Table 1 contains the worksheet data from Appendix A. All salt solutions were identified with the exception of solution A. When observing the light emitted from solution A, no consensus was reached as to the colour of light emitted. Results ranging from red, red/orange and red/pink were suggested, and red/pink was decided to be the closest colour to what was observed. However, without a consensus as to the colour of light emitted, no viable identification of the metal salt contained in the solution could be made.

Solution H was identified as containing Sodium and Potassium through the use of the Cobalt glass. This eliminated the orange wavelength light from the Sodium emission spectra and clearly showed the lavender wavelength light from the Potassium cations.

As discussed above, despite a lengthy discussion with peers, solution A remained unidentified due to the subjectivity of identifying colours of light emitted using only visual observation. This subjectivity can be removed through the use of an optical spectrograph that can quantize the observed wavelengths. Further sources of error may be attributed to: the lighting of the room not being controlled (including the sunlight through the windows), cross-contamination despite the cleaning step 3 of the method (e.g. inadequate cleaning of the Nichrome wire loop, the Bunsen burner chimneys collecting detritus over prolonged use), and potentially due to the group consisting only of adult males. There is evidence to suggest that males are less capable than females of distinguishing between the colour spectrum, particularly on the red-green axis, potentially due to retinal physiology and also are less able to correctly verbalize the observed colour [12].

Table 2 contains the energy calculations from the observed data. The subjectivity in the method is highlighted by the closeness of wavelengths between Calcium's orange flame of 600nm and Strontium's red flame of 650nm. The results demonstrate the relationship between wavelength decreasing as energy of the photon and subsequently frequency in Figure 6.

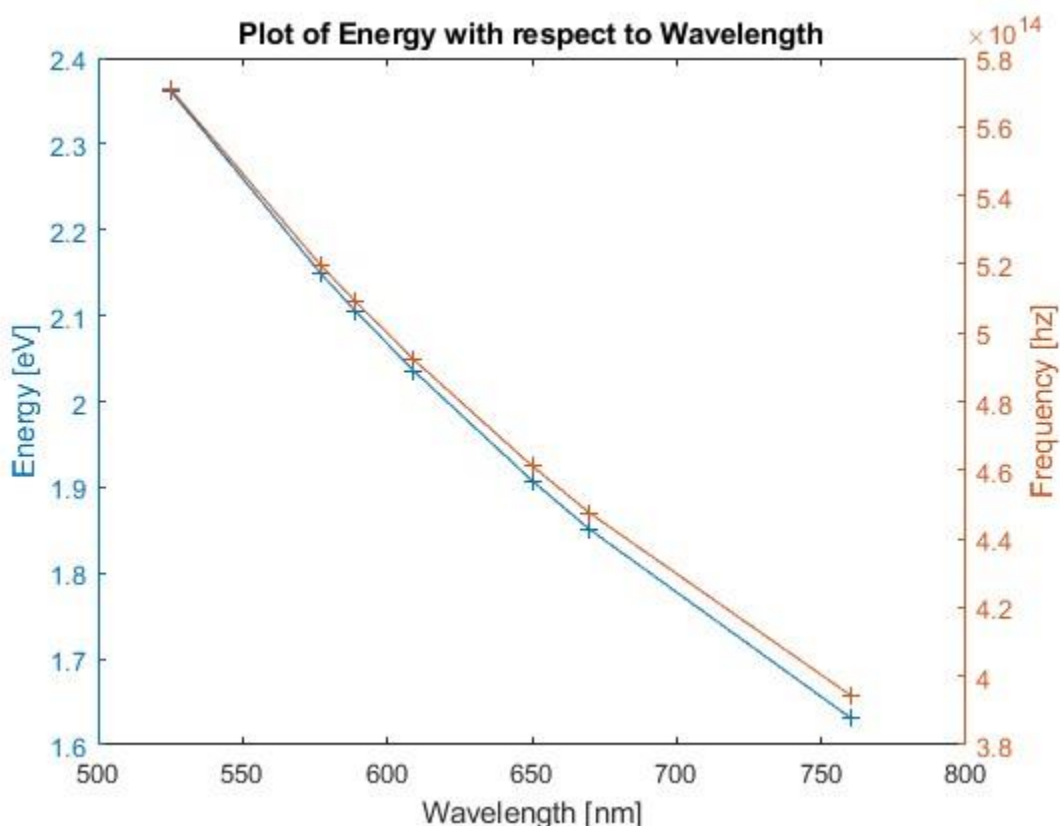


FIGURE 4 - PLOT OF ENERGY WITH RESPECT TO WAVELENGTH

Table 3 contains wavelengths taken from spectrograph measurements [11] to calculate more accurate photon energy data.

CONCLUSION

The component elements of the unknown metal salt solutions were identified by observing the light emitted upon heating of the solutions, and comparing the results to known emission spectra. While visual inspection was used with reasonable success, the inherently subjective nature of visual results, as well as the lack of precision, led to difficulty in identifying solution A. Further sources of error within the experiment were also considered. To obtain more repeatable and accurate results, use of measuring instruments such as an optical spectrometer can more accurately and precisely measure the wavelength of light emitted by the solution when heated.

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APPENDICES

APPENDIX A

University of Wales Trinity Saint David – OME Programme

DATA SHEET to RECORD OBSERVATIONS, CALCULATIONS and RESULTS

date 02/06/23

STUDENT'S NAME: TOM VOLPATO & ALEX HALLIDAY

Observations and Identification:

(9p) Complete the table below. Based on the observed colour of the flame and Table 1, identify the metal ion in each unknown salt. Using the electromagnetic spectrum in Fig 2, estimate and report with the appropriate unit the wavelength for each observed colour.

Identify the solution containing mixture of sodium and potassium:

Unknown metal salt	Colour of the flame	Identity of metal	Wavelength nm
DI water	ORANGE	-----	-----
1 M HCl		-----	-----
A GLASS	RED ORANGE RED/PINK NA (yellow flame)	INCONCLUSIVE ← SODIUM	700
B GLASS	RED/PINK RED	STRONTIUM	650
C G	ORANGE ORANGE	CALCIUM	600
D G	VIOLET VIOLET	BARIUM ?	400
E G	YELLOW YELLOW	~~SODIUM~~	580
F G	RUBY RED NA (yellow flame)	LITHIUM	700
G G	GREEN / BLUE GREEN	COPPER	500 - 550
H G	ORANGE LAVENDER	POTASSIUM + SODIUM	600 400 - 450

If in doubts refer to literature/youtube/etc

APPENDIX B

POTENTIAL HAZARD

Chemical	Hazards
Hydrochloric acid solution (1 M HCl)	 Causes severe skin burns and eye damage.  Harmful if swallowed.
Barium chloride (BaCl_2)	 Acute toxicity (oral, dermal, inhalation), category 3.  Irritant.
Calcium chloride (CaCl_2)	 Causes serious eye irritation.
Lithium chloride (LiCl)	 Causes serious eye irritation.  Harmful if swallowed.  Causes skin irritation.
Strontium chloride (SrCl_2)	 Serious eye damage.
Strontium nitrate ($\text{Sr}(\text{NO}_3)_2$)	 May intensify fire; oxidiser  Harmful if swallowed. Causes serious eye irritation. Can cause respiratory irritation
Potassium chloride (KCl)	 Causes serious eye irritation.
Potassium nitrate (KNO_3)	 May intensify fire; oxidiser
Sodium chloride (NaCl)	Not classified as a hazardous chemical
Copper chloride (CuCl_2)	 Harmful if swallowed or in contact with skin.  Causes skin irritation and serious eye damage.  Very toxic to aquatic life wilong-lasting effects.

APPENDIX C

Matlab plotting script for Figure 6:

```
clc
clear all

dataset = xlsread('LabReport Calcs.xlsx','Sheet1',['I2:k8'])
x = dataset(:,1);
y = dataset(:,2);
yy = dataset(:,3);

yyaxis left
plot(x,y,'-+')
title(['Plot of Energy with respect to Wavelength'])
xlabel('Wavelength [nm]')
ylabel('Energy [eV]')

yyaxis right
plot(x,yy,'-+')
ylabel('Frequency [hz]')
```