

Research Question

How does the ligand's relative position to H₂O in the spectrochemical series affect the light absorbency of octahedral coordination complexes between metal cations and ligands in 6 different metals: copper, iron, nickel, zinc, cobalt, and silver?

Introduction

During IB chemistry class, I have learnt about how transition metals can form coloured complexes, unlike other metals, with a species called ligands. However, my curiosity in how the different positions in the spectrochemical series may affect the colour of different transition metals was not able to be solved only with the IB curriculum. I became especially interested in how the electrons can be promoted between d orbitals with different amounts of energy. The time allowed to investigate this topic was limited in chemistry class, therefore, I decided to further investigate the Crystal Field Theory and how this may be recreated in the lab.

Aim

This discussion's aim is to explore the relationship between the ligands' position in the spectrochemical series and the light absorbency of octahedral coordination complexes in copper, iron, nickel, zinc, cobalt, and silver using solutions of each metal. Ligands will be added to each metal solution and observe the colour, and since different colours would show different light absorbencies, this will be measured using a colorimeter.

Background Knowledge

The mechanism of observing colour

As white light passes through a coloured solution, some range of wavelengths in the light are absorbed, while others are reflected and this is why our eyes can perceive different colours. For example, if the light passes through a red coloured solution, it will absorb the wavelengths in the blue region of the light spectrum, while reflecting the wavelengths in the red region of the light spectrum. The reflected wavelengths will arrive to our eyes which will translate the wavelength to colour together with the brain.

Beer-Lambert Law

$$A = \epsilon lc$$

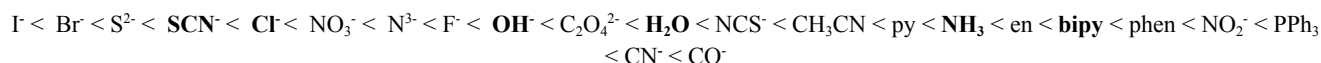
Beer-Lambert Law is the equation above which relates the molar concentration of a solution to the absorbance. Here, A is the absorbance of the solution, ϵ (epsilon) is the molar absorptivity: how well the substance absorbs light, l is the distance that light travels through the solution, and c is the concentration of the solution. This equation is frequently used in spectroscopy since it measures the absorbance of a light at a specific wavelength.

Transition Metals

Transition elements are located on the d-block of the periodic table. They are characterised by having partially filled d-orbital. Therefore, zinc(Zn²⁺) is not considered as a transition metal since it has a full 3d subshell - the electron configuration of zinc ion is 3d¹⁰ 4s⁰. In most of the cases, electrons occupy the 4s subshell first then 3d subshell. However, copper(Cu) and chromium(Cr) atoms are exceptions. Chromium and copper atoms have just one electron in the 4s subshell because having 5 electrons in the 3d subshell is more stable than having full 4s electrons and having 4 electrons in the 3d shell. The partially filled d orbital leads to several attributes of transition metals such as variable oxidation states, catalytic activity and forming coloured complexes.

Ligands and the Spectrochemical Series

Complexes are made up of central metal ions encompassed by ions or molecules which form coordinate covalent bonds (dative covalent bonds). Ligands are species that donate their lone pairs to chemically bond with the central transition metals, which indicates that they are all Lewis bases. They can be both negative - SCN^- and Cl^- - or neutral - NH_3 and H_2O . These examples are called as unidentate or monodentate since each ligand donates one electron pair to the transition metal. Ligands also can be bidentate, which donate two lone pairs of electrons. The colour of the complexes often change depending on the position of the ligand on the spectrochemical series.

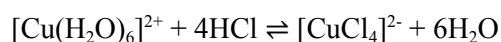


This is the spectrochemical series that I have used. The right side has shorter wavelength, which would induce greater absorption of energy; the left side has longer wavelength, which would induce less absorption of energy.

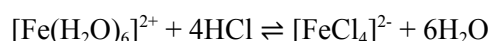
Ligand Exchange Reaction in this Experiment

These are the ligand exchange reactions that happened during the experiment between water ligands and other ligands. The followings are examples for each transition metal, where H_2O ligands are replaced with Cl^- ligands.

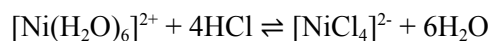
1. Cu^{2+}



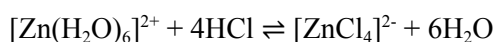
2. Fe^{2+}



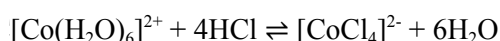
3. Ni^{2+}



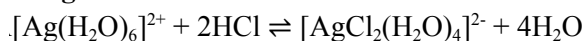
4. Zn^{2+}



5. Co^{2+}



6. Ag^+



Crystal Field Theory and Octahedral Coordination Complexes

Crystal field theory (CFT) is a model that explains the behaviour of transition metal ions in coordination compounds and according to CFT, when a transition metal ion bonds with a set of ligands, the ligands create a crystal field that splits the d-orbitals with the same energy - degenerate - of the metal ion to different energy levels. Depending on the geometry of the ligands around the metal ion, the splitting of d-orbital changes. In octahedral coordination complexes, which this exploration will focus on, the ligands are arranged in an octahedral geometry.

The colour of complex ions - including the octahedral complex - comes from the repulsion of electrons between the ligands and transition metal ions. Two d orbitals lie along the xyz axis, and three of the 3d orbitals lie between the axes as shown in Figure 1.2. (chemtalk). Ligands approach along the axes so the ligands repel electrons in orbitals on the axes more. As a result, 2 orbitals have higher energy than the other 3 orbitals. Therefore, this splits the 6 d orbitals into 2 distinct energy levels. When electrons are promoted from the lower energy level d-orbital to higher energy level d-orbital - which is called d-d transition - energy is absorbed. The amount of energy gap between d orbitals decides the wavelength of the light that will be absorbed. This is shown through the equation $\Delta o = hc/\lambda$. Here, Δo is the energy absorbed when an electron is promoted to the higher energy level d orbital, h and c are constants, and λ denotes the wavelength. After the electron is promoted, it comes back to its original state by releasing energy. This process is why observed colour sometimes changes or fluorescence in some coordination compounds when they absorb and release energy.

The following diagram shows the 'colour wheel'. Here, the colours that are positioned opposite to each other (e.g. red and cyan) are complementary to each other. If the wavelength absorbed is included in the region of certain colour of the wheel, the complementary colour will be visible to our eyes.

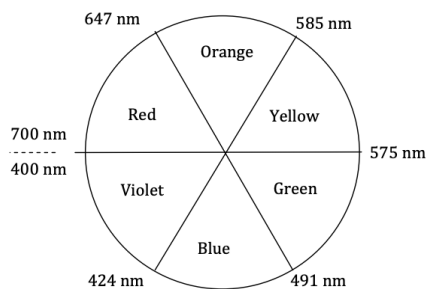


Figure 1.1. Colour Wheel Showing Complementary Colours(data booklet)

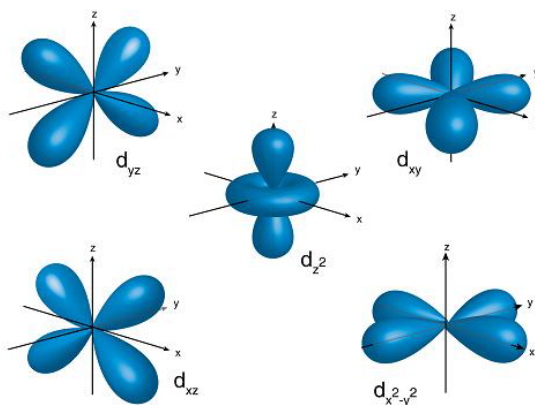


Figure 1.2. Arrangement of d orbitals(chemtalk)

In figure 1.3.(chemguide), since yellow light is absorbed, the complementary colour of yellow, which is dark blue, will be shown.

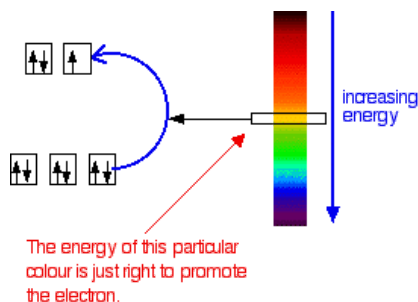


Figure 1.3. Correspondence between energy gap between d orbitals and light spectrum(chemguide)

Just like different transition metal cations show different colours, different types of ligands and number of ligands exhibit different complementary colours. The colour of a complex depends on the magnitude of which depends on the structure of the complex, because the Δ_o of a photon is inversely proportional to its wavelength. The compound $[\text{Cr}(\text{NH}_3)_6]^{3+}$, for instance, contains strong-field ligands and large Δ_o . It exhibits a yellow colour since it absorbs relatively high-energy photons, which correspond to blue-violet light. On the other hand, the $[\text{Cr}(\text{H}_2\text{O})_6]^{3+}$ ion, a compound with the same central metal cation but weaker-field ligand, absorbs lower-energy photons associated with the yellow-green region of the visible spectrum, giving it a complementary colour of dark violet shade.

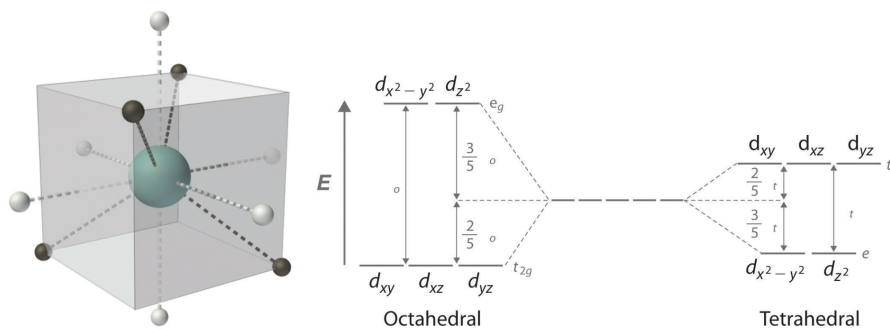


Figure 1.4. Splitting of d Orbitals in Octahedral and Tetrahedral Complexes

In the tetrahedral complex, four ligands are bonded to the central metal cation, and d orbitals are split into 2 distinct energy levels. d_{xy} , d_{xz} , and d_{yz} orbitals are placed on the top since they have higher energy, while $d_{x^2-y^2}$ and d_{z^2} orbitals are placed on the bottom since they have lower energy levels. Conversely, in the octahedral complex, $d_{x^2-y^2}$ and d_{z^2} orbitals have lower energy levels than that of d_{xy} , d_{xz} , and d_{yz} orbitals. As seen in the figure, the gap between higher energy level and lower energy level d-orbitals in the octahedral complex is larger compared to the tetrahedral complex. Greater gap suggests that energy change is greater when the electrons are promoted from the lower energy d-orbital to the higher energy d-orbital.

An example of an octahedral coordination complex ion is $[\text{Al}(\text{H}_2\text{O})_6]^{3+}$, which is shown in figure 1.4. Here, Al^{3+} ion is the central transition metal ion and 6 H_2O molecules act as ligands. In order to form this ion, Al^{3+} ion is dissolved in water. Figure 1.5. shows the shapes of transition metal-ligand complexes with the example of Cu^{2+} .

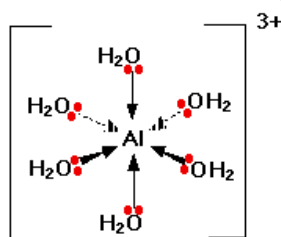


Figure 1.4. Complex ion $[\text{Al}(\text{H}_2\text{O})_6]^{3+}$ formed by OH_2 donating a lone pair to Al^{3+} transition metal. Arrows indicate dative covalent bonds formed between them.(chemguide)

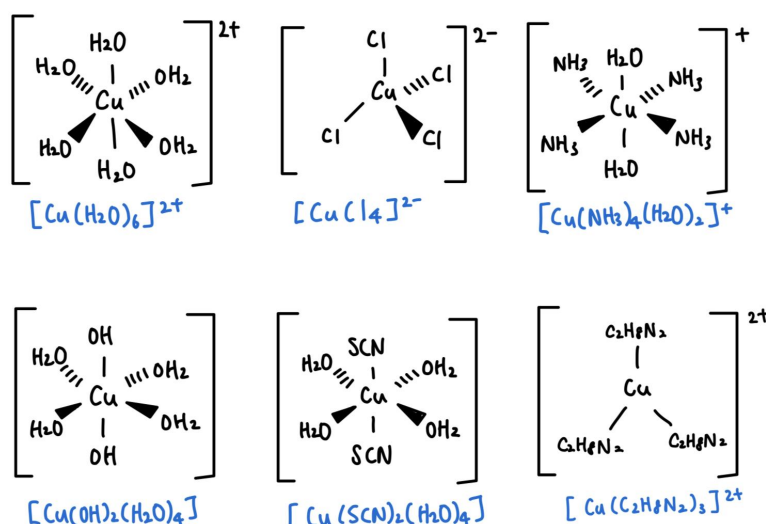


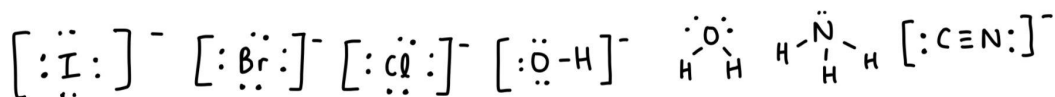
Figure 1.5. Diagram of transition metal complex ion Cu^{2+} and its shape with 6 different ligands that will be used in this experiment

Variables

Independent Variable:

The independent variable is the extent of d-orbital splitting and this will be manipulated depending on the type of transition metal ions and position of the ligands in the spectrochemical series.

- Position of the ligands in the spectrochemical series
- Iodine(I⁻), bromine(Br⁻), chloride(Cl⁻), hydroxide(OH⁻), thiocyanate(CN⁻), ammonia(NH₃)
I⁻ < Br⁻ < Cl⁻ < OH⁻ < H₂O < NH₃ < CN⁻ < bipy



- Type of transition metal ions
- Copper sulphate(CuSO₄), iron chloride(FeSO₄), nickel sulphate(NiSO₄), zinc sulphate(ZnSO₄), cobalt chloride(CoCl₂), silver nitrate(AgNO₃)

Dependent Variable:

The dependent variable is the light absorbance of octahedral coordination complexes in a variety of metal complex ions, which will be measured by a colorimeter.

Control Variables:

	Reason of control	Method of controlling
Concentration of metal salts and ligands (mol dm ⁻³)	If the concentration of salts and ligands are different, different amounts of complexes would be formed.	All prepared metal solutions and ligands were made to be 0.1 mol dm ⁻³
Volume of metal solution and ligand used	Higher/lower amount of ligand would result in a shift in the position of equilibrium.	Use a volumetric pipette to measure each 5 ml and 10 ml of metal solution and ligand.
Wavelength range used for the colorimeter	The wavelength of the metal solutions may not be measured due to not being in the range	Wavelength of 700nm was used throughout the experiment.
Type of ligands used for each metal solution	Different ligands will cause different d orbital splitting, which would not allow comparison between the ligand and wavelength absorbed.	For each metal solution, I used 6 different ligands.
Type of colorimeter	Different colorimeters might be calibrated differently and give a different wavelength.	I used a vernier colorimeter for all metal cation + ligand solutions.

Preliminary Experiment

Finding the right revolutions per minute(RPM) for the magnetic stirrer

Magnetic stirrer needs to be used correctly since too high RPM will cause splashing of the solution to the surrounding which is hazardous and would waste the chemicals. Therefore, after a few initial trials, I concluded that 400 RPM is the most appropriate speed.

Finding the volume ratio for metal solution and ligands

Appropriate ratio between metal solution and ligand must be used in order to observe clear colour change. I used a volumetric pipette to see how much ligand was required to observe the colour change in the metal solution. The ratio of 1:2, that is, $5\text{cm}^3 : 10\text{cm}^3$ was found to be suitable.

Finding the suitable wavelength in colorimeter

Since most complexes showed green to blue colour and some had red colour range, I chose the wavelength of 700 nm. Because this shows the absorption of red in the colour wheel, most complexes will exhibit an appropriate range of absorbance values.

Methodology

Apparatus

Metal/Ligand Solution	Volume	Concentration	Equipment	Quantity	Uncertainty
$\text{CuSO}_4(\text{aq})$	5.00 ml	0.10 mol dm^{-3}	Magnetic stirrer	1	N/A
$\text{FeCl}_3(\text{aq})$	5.00 ml	0.10 mol dm^{-3}	Automatic pipette	1	$\pm 0.01 \text{ ml}$
$\text{NiSO}_4(\text{aq})$	5.00 ml	0.10 mol dm^{-3}	40 ml beaker	8	$\pm 5.00 \text{ ml}$
$\text{ZnSO}_4(\text{aq})$	5.00 ml	0.10 mol dm^{-3}	Plastic pipettes	12	N/A
$\text{CoCl}_2(\text{aq})$	5.00 ml	0.10 mol dm^{-3}	Colorimeter	1	N/A
$\text{AgNO}_3(\text{aq})$	5.00 ml	0.10 mol dm^{-3}			
$\text{NH}_3\text{OH}(\text{aq})$	10.00 ml	0.10 mol dm^{-3}			
$\text{NaOH}(\text{aq})$	10.00 ml	0.10 mol dm^{-3}			
$\text{KSCN}(\text{aq})$	10.00 ml	0.10 mol dm^{-3}			
$\text{C}_2\text{H}_8\text{N}_2(\text{aq})$ (ethylenediamine)	10.00 ml	0.10 mol dm^{-3}			
$\text{HCl}(\text{aq})$	10.00 ml	0.10 mol dm^{-3}			

General procedure of using colorimeter to measure the absorbance of aqua complex ions

1. Calibrate the colorimeter following the procedure written on the box.
2. Ensure the cuvettes are clean.
3. Fill up roughly $\frac{2}{3}$ of the cuvettes with the metal solutions using a pipette.
4. Place the cuvette correctly in the colorimeter (smooth side facing the light source).
5. Ensure the colorimeter is set to the correct wavelength
6. Record the wavelength of light absorbance
7. Remove the cuvette and reset the colorimeter to attain the average to minimise random error

Making transition metal complexes

1. Measure 5 ml of copper sulphate solution using an **automatic pipette** and pour this in the 40 ml beaker. For greater accuracy, make sure there aren't any air bubbles and remove the thumb completely from the

controller button once it reaches the home position.

- Add the ligand by the ratio of: $\frac{2}{3}$ metal solution by volume and $\frac{1}{3}$ ligand, which is 10 ml of ammonia into the beaker. Measure 10 ml with an **automatic pipette**.
- Place the beaker with metal solution on the magnetic stirrer and submerge the magnetic flea in the solution.
- Set the power as 400 RPM and let it spin for 10 seconds to mix the metal solution and ligand.
- Pick out the magnetic flee by the piece of magnet from the beaker
- Fill the $\frac{2}{3}$ of the cuvette with the copper sulphate + ammonia ligand solution using a pipette
- Measure the wavelength of light absorbance using a colorimeter. Refer to the procedure above. Repeat this for 3 times to minimise random error that can happen when using a colorimeter.
- Repeat the same for each additional ligand (NaOH, SCN, C₂H₈N₂, HCl)
- Repeat the steps 1 - 8 for each additional stalk metal solution (FeSO₄, NiSO₄, ZnSO₄, CoCl₂, AgNO₃)
- Repeat 3 readings for each one and average the data.

Risk Assessment

There aren't any environmental factors or ethical factors.

Chemical	Hazards	How to prevent
Solvents such as NaOH and HCl: may be flammable, toxic, or irritant	Fire hazard: flammable solvents may ignite if exposed to heat or flame	Keep flammable solvents away from the heat sources
Metal salts and ligands: may be toxic, corrosive, or irritant depending on the type and concentration	Chemical hazards: exposure to toxic, corrosive, irritant chemicals may cause harm to human health or the environment	Wear PPE(personal protective equipment) such as lab coat, gloves, and safety goggles

Raw Data

	Absorbance at wavelength 700 nm in different metal solutions						
Ligand	Result	Cu ²⁺	Fe ²⁺	Ni ²⁺	Zn ²⁺	Co ²⁺	Ag ⁺
H₂O	Colour change	blue	light yellow	green	Colourless	Pale pink	Colourless
	Reading	1. 0.739 2. 0.729 3. 0.740	1. 0.466 2. 0.496 3. 0.470	1. 0.481 2. 0.484 3. 0.494	1. 0.437 2. 0.438 3. 0.439	1. 0.023 2. 0.024 3. 0.023	1.0.012 2.0.011 3. 0.010
	Average	0.736	0.477	0.486	0.438	0.0233	0.011
NH₃OH	Colour change	cloudy lighter blue	pale yellow	no change	cloudy	emerald green	no change
	Reading	1. 0.762 2. 0.755 3. 0.700	1. 0.457 2. 0.456 3. 0.457	1. 0.458 2. 0.456 3. 0.458	1. 0.436 2. 0.441 3. 0.446	1. 0.005 2. 0.005 3. 0.005	1.-0.001 2.-0.002 3. -0.001
	Average	0.739	0.457	0.457	0.441	0.005	-0.00133
NaOH	Colour change	cloudy lighter blue	orange	no change	no change	pale purple	turbid yellow
	Reading	1. 0.888	1. 0.507	1. 0.541	1. 0.451	1. 0.006	1.1.410

		2. 0.822 3. 0.800	2. 0.508 3. 0.507	2. 0.540 3. 0.539	2. 0.453 3. 0.451	2. 0.005 3. 0.005	2.1.440 3. 1.453
	Average	0.837	0.507	0.54	0.452	0.00533	1.43
KSCN	Colour change	green blue	brick red	no change	no change	no change	white
	Reading	1. 1.007 2. 1.0103 3. 1.011	1. 0.521 2. 0.525 3. 0.523	1. 0.920 2. 0.920 3. 0.920	1. 0.511 2. 0.509 3. 0.512	1. 0.095 2. 0.096 3. 0.096	1.1.826 2.1.813 3. 1.832
	Average	1.009	0.523	0.92	0.511	0.096	1.824
C₂H₈N₂	Colour change	dark navy	orange	Light purple	no change	brown	pale yellow
	Reading	1. 0.698 2. 0.697 3. 0.699	1. 0.478 2. 0.479 3. 0.477	1. 0.448 2. 0.448 3. 0.447	1. 0.418 2. 0.418 3. 0.418	1. -0.003 2. -0.003 3. -0.004	1.-0.001 2.-0.001 3. -0.001
	Average	0.698	0.478	0.448	0.418	-0.00333	-0.001
HCl	Colour change	green	yellow	no change	no change	no change	white
	Reading	1. 0.954 2. 0.950 3. 0.949	1. 0.496 2. 0.495 3. 0.510	1. 0.451 2. 0.452 3. 0.453	1. 0.447 2. 0.449 3. 0.450	1. 0.007 2. 0.007 3. 0.007	1.1.824 2.1.833 3.1.832
	Average	0.951	0.5	0.452	0.449	0.007	1.830

Percentage Error Calculation

e.g.) [Cu(H₂O)₆]²⁺ complex

Percentage uncertainty(un.) of volume measurement

$$= \left(\frac{\text{un. of burette}}{\text{Vol. from initial trial}} + \frac{\text{un. of automatic pipette}}{\text{Vol. of metal solution}} + \frac{\text{un. of automatic pipette}}{\text{Vol. of ligand solution}} \right) \times 100$$

$$= \left(\frac{0.05}{10.00} + \frac{0.01}{5.00} + \frac{0.01}{10.00} \right) \times 100$$

$$= 0.8\%$$

Percentage uncertainty (un.) of the average absorbance value

$$= \left(\frac{\text{un. of colorimeter measurement}}{\text{absorbance in 1st trial}} + \frac{\text{un. of colorimeter measurement}}{\text{absorbance in 2nd trial}} + \frac{\text{un. of colorimeter measurement}}{\text{absorbance in 3rd trial}} \right) \times 100$$

$$= \left(\frac{0.0005}{0.698} + \frac{0.0005}{0.697} + \frac{0.0005}{0.699} \right) \times 100$$

$$= 0.215\%$$

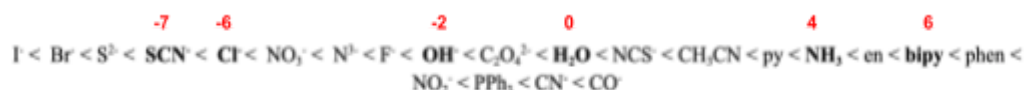
$$\text{Total percentage uncertainty} = 0.8 + 0.215 = 1.015\% \approx 1\%$$

$$\rightarrow \text{Uncertainty} = 0.698 \times \frac{1}{100} = \pm 0.00698 \approx \pm 0.007$$

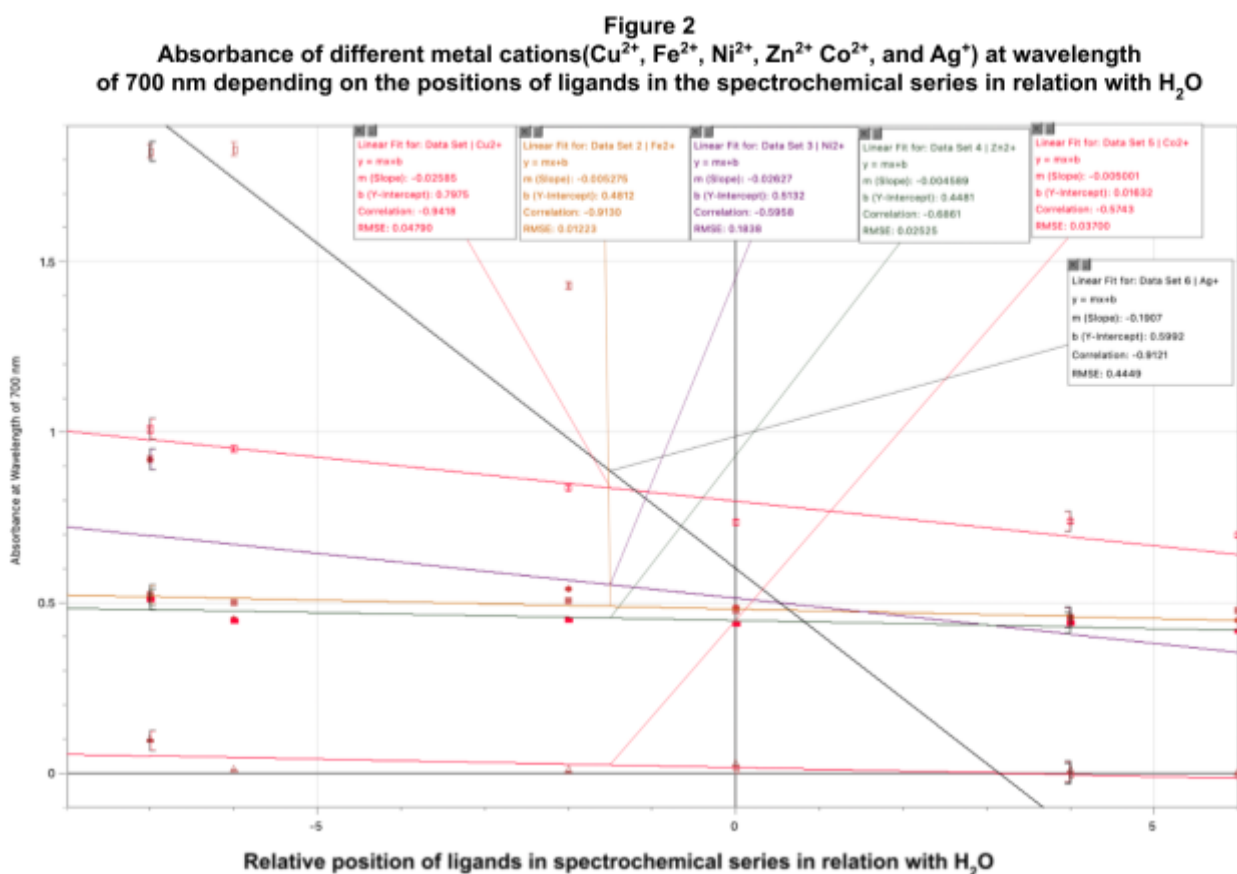
Organised Data

	Mean absorbance at wavelength 700 nm in each metal solutions (\pm uncertainty)					
Ligand (Relative position to water)	Cu^{2+}	Fe^{2+}	Ni^{2+}	Zn^{2+}	Co^{2+}	Ag^+
KSCN (-7)	1.009 \pm 0.01	0.523 \pm 0.005	0.92 \pm 0.009	0.511 \pm 0.005	0.096 \pm 0.001	1.82 \pm 0.02
HCl (-6)	0.951 \pm 0.01	0.5 \pm 0.005	0.452 \pm 0.005	0.449 \pm 0.004	0.007 \pm 0.00007	1.83 \pm 0.02
NaOH (-2)	0.837 \pm 0.008	0.507 \pm 0.005	0.54 \pm 0.005	0.452 \pm 0.005	0.00533 \pm 0.00005	1.43 \pm 0.01
H_2O (0)	0.736 \pm 0.007	0.477 \pm 0.005	0.486 \pm 0.005	0.438 \pm 0.004	0.0233 \pm 0.0002	0.01 \pm 0.0001
NH_3OH (+4)	0.739 \pm 0.007	0.457 \pm 0.005	0.457 \pm 0.005	0.441 \pm 0.004	0.005 \pm 0.00005	-0.0013 \pm 0.00001
$\text{C}_2\text{H}_8\text{N}_2$ (6)	0.698 \pm 0.007	0.478 \pm 0.005	0.448 \pm 0.004	0.418 \pm 0.004	-0.00333 \pm 0.00003	-0.001 \pm 0.00001

To create calibration curves from these data, each ligand species was given a value that represented where it is placed in the spectrochemical series in relation to water. After that, the values were plotted using Logger Pro. Each linear line for different metal cations are colour coded.



This graph shows the correlation between the relative position of ligands in spectrochemical series in relation with H_2O . Each metal complex is colour coded and the boxes on the top show the slope of the line. Although error bars are drawn with uncertainty, the error bound is insignificantly small therefore is disregarded.



As seen in figure 2, Cu^{2+} data (red line) clearly exhibits a decreasing slope in absorbance from the ligand position of -7 to 6. Likewise, Ni^{2+} (purple line) has a similar negative slope with Cu^{2+} and has a clear decreasing trend throughout increasing positions of ligands in spectrochemical series. Fe^{2+} (yellow line), Zn^{2+} (green line), and Co^{2+} (red line) data, on the other hand, has a negative slope but is very weak with the slope about $-0.00528(3.s.f.)$, $-0.00459(3.s.f.)$, and $-0.191(3.s.f.)$. This can be inferred by the qualitative data, where the colour change was insignificant or didn't change drastically as much as expected. Ag^+ (black line) showed the greatest change in absorbance wavelength at 700 nm throughout the ligands in spectrochemical series. This can be inferred from the qualitative data where the opaqueness changed drastically from colourless to white.

Conclusion and Discussion

Copper(Cu^{2+}) Complexes - Red Line

According to the Cu^{2+} data's trend, as the position of ligands in the spectrochemical series increases - which means increase in energy level - the absorbance of wavelength in 700 nm by the ligands decreases. This is coherent with the equation $\Delta o = hc/\lambda$, where energy (Δo) of a light particle, photon, is inversely proportional to wavelength (λ).

However, the correlation is very weak with the data points deviating from the trend line. The data point with ligand H_2O , the absorbance of wavelength in 700 nm is lower compared to the expected value and the trend line. In one perspective, this may be due to aqueous Cu^{2+} having lower absorbance compared to other data points, but it may be due to the other data points being higher. As seen in the qualitative data, Cu^{2+} octahedral complexes form cloudy precipitation. This would eventually disrupt the absorbance value during colorimeter measurement.

Iron(Fe^{2+}) Complexes - Yellow Line and Zinc(Zn^{2+}) Complexes - Green Line

Fe^{2+} data generally exhibits decreasing trend with the slope of $-0.00526(3.s.f.)$, but the trend is very weak therefore cannot be said that there is a significant change by changing the ligands' position on the spectrochemical series.

Likewise, the Zn^{2+} data also exhibits an extremely weak trend with the slope of $-0.00459(3.s.f.)$. The data variation is less than 0.1 despite the apparent colour change. Moreover, the trend line is all included in the boundaries of the error bar, which suggests that the gradient is not significant.

The main reason for this tenuous trend is because the extent of d-orbital splitting is not big enough to be seen clearly in terms of the wavelength. The absorbance at a certain wavelength largely depends on the extent of d-orbital splitting. Greater energy gap between the higher energy level d-orbitals and lower energy d-orbitals leads to greater absorbance. However, because the energy gap between d-orbitals are generally small and they don't vary much, the absorbance is also generally low and the change is indiscernible.

Nickel(Ni^{2+}) Complexes - Purple Line

Ni^{2+} displays a decreasing trend of absorbance at wavelength at 700 nm. As the position of ligands in the spectrochemical series increases, the splitting of d-orbital increases, which also increases the energy gap between the d-orbitals. This leads to the absorbance of shorter wavelengths. This also corresponds to the definition of energy, which is $\Delta o = hc/\lambda$.

One characteristic of the qualitative data of Ni^{2+} was that the colour change was unrecognisable. Except the $[\text{Ni}(\text{en})_3]^{2+}$ complex - which had light purple colour - the rest of the complexes were the same with the aqueous solution of Ni^{2+} . However, the absorbance differed. This may be accounted for by the initial complex formation of Ni^{2+} with other ions rather than H_2O in the solution. The presence of impurities would alter the colour of the complex and even change the shape of the complex. Therefore, different splitting showed and as a result exhibited colour change indiscernible to our eyes.

Cobalt(Co^{2+}) Complexes - Pink Line

Co^{2+} data, like other data, shows decreasing absorbance at wavelength of 700 nm depending on the position of ligand on the spectrochemical series. One characteristic is that all absorbance values are very close to 0. This suggests that the d-orbital splitting is very slight, therefore we can infer that the ligand-field splitting is weak. Weak-field ligands don't induce significant splitting of the d-orbitals, therefore the energy gap between lower and higher energy d-orbital is limited. Therefore, there is a low probability of electronic transitions that could absorb photons. Another possible explanation is that there are no suitable transitions. Due to the insignificant energy gap between high and low level of d-orbitals, which means that transitions available are of low energy and this corresponds to the absorption of wavelengths in the near-UV regions of light spectrum. This has the probability of being beyond the colorimeter's measurements which leads to absorbance values that appear to be close to 0 in the visible region.

Silver(Ag^{2+}) Complexes - Black Line

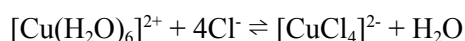
Ag^+ data shows the trend most clearly among all complexes, where the gradient is greatest with the value of -0.197. Ligands ranked higher in the spectrochemical series brought less absorbance of wavelength at 700 nm, which corresponds with the equation $\Delta o = hc/\lambda$ where higher energy leads to decreased wavelength.

However, this clear trend can be accounted for by the presence of precipitation, which altered the absorbance of wavelengths in the colorimeter. As seen in the qualitative table, a few had intransparent colours, which suggests the presence of precipitation. This is not considered in the equation of $\Delta o = hc/\lambda$, therefore, needs to be considered a limitation.

Evaluation

Generally, the error bars were negligible and control variables were kept constant without significant error. However, there are some overall errors that impacted my results:

- Some of the metal ions + ligand complexes didn't form complete octahedral complexes, due to the large size of the ligand atoms. For example, when HCl was added to aqueous Cu^{2+} , it is likely that they had formed tetrahedral complexes like the following equation:



- Some methodological limitations were present, too; they are listed in the table below.

Method	Limitation	Direction of Error	Mitigation
Colorimeter measurement	When ligand was added to the aqueous metal solution, undissolved precipitation formed in the cuvette for some octahedral complexes such as $[\text{Cu}(\text{NH}_3)_6]^{3+}$ and $[\text{Zn}(\text{NH}_3)_6]^{3+}$. The cuvette became cloudy or stale.	The absorbance of the salt is not supposed to be included in the absorbance. The precipitation formed may have hindered the light passing through the cuvette, therefore might have disrupted the absorbance value in wavelength of 700 nm. Specifically, it would <u>increase the absorbance</u> . For example, $[\text{Cu}(\text{NH}_3)_6]^{3+}$ and $[\text{Cu}(\text{H}_2\text{O})_4(\text{OH})_2]$ both had cloudy colour, and had slightly higher absorbance value than the trendline.	The solid should be decanted or wait until the salt all sinks down on the bottom of the cuvette. This will prevent the precipitation from hindering the light passing through the colorimeter. Alternatively, excess ligands may be used in order to fully dissolve the salts.
Controlling	The temperature of the	When temperature decreases, the	Use a water bath to keep the

conditions	surrounding area was not controlled or kept constant.	equilibrium constant of the reaction also changes. This would alter the number of moles of coloured compounds formed. For example, $\text{Fe}^{2+} + \text{HCl}$'s forward reaction is exothermic. When temperature decreases, the equilibrium will shift to the right and increase the amount of complex formed and when temperature increases, the equilibrium will shift to the left and decrease the amount of complex formed.	solutions and ligands' temperature constant. Also, do not turn the air conditioner on and off during the experiment, and keep it at a constant room temperature of 26 degrees celsius.
	The water used in order to make ligand solution was distilled water, which contains various mineral ions and cations.	The ions could hinder or disrupt the displacement process of ligand species. This may result in exhibition of 'mixed' colour complexes. Other ions instead of the ligand may have replaced the H_2O and show inaccurate colour.	Use deionized water, if available. This has no other elements than H and O therefore there is no possibility of H_2O getting displaced by other minerals present in distilled water.
Ligand exchange	$[\text{Cu}(\text{H}_2\text{O})_6]^{2+} + 4\text{HCl} \rightleftharpoons [\text{CuCl}_4]^{2-} + 6\text{H}_2\text{O}$ <p>Although a preliminary experiment was held in order to find the suitable ratio between metal solution and ligand, 5:10 cm^3 was not enough to replace the H_2O ligand fully. Therefore, some ligands might have gone through incomplete exchange, instead of fully displacing H_2O.</p>	Incomplete exchange of ligand will affect the splitting of d orbitals. Fully exchanged ligands would have different splitting differences compared to the partially exchanged ligands. This would result in exhibition of different colours as well as different absorbance at wavelengths of 700 nm.	Apparently, the preliminary experiment was not enough. Therefore, I should conduct more steps in the preliminary experiment until the colour change is not visible and pour excess ligands.

Further Investigation

- Instead of using positions of ligand relative to H_2O as the x axis of the graph, other measurements can be used. For example, the literature values for the ligands' splitting energy of a metal ion could be used as a scale.
- In order to dissolve the precipitation or salt produced in the metal solution + ligand, excess ligand is needed. Further investigation about exactly how much is needed to make the complex clear of precipitation can be held. Moreover, the minimal concentration of ligands needed in order to form a metal ion-ligand complex can also be studied.
- Instead of changing the ligands, the independent variable can be changed. One example would be comparing the absorbance at wavelength of 700 nm between octahedral complexes(e.g. $[\text{Cu}(\text{H}_2\text{O})_6]^{2+}$), tetrahedral complexes(e.g. $[\text{CuCl}_4]^{2-}$), and linear complexes(e.g. $[\text{Cu}(\text{CN})_2]^{2-}$). Another example would be investigating the effect of charge on the central metal ion on the extent of d-orbital splitting.

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