INVESTIGATION OF THE EFFECT OF NATURE OF LIGAND ON THE CRYSTAL FIELD SPLITTING PARAMETER OF OCTAHEDRAL CHROMIUM(III) COMPLEXES

Extended Essay in Chemistry HL

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ABSTRACT

Transition metal complexes are mostly coloured. These colors are known to be resulted from the energy difference between the sperated d-shells. The amount of seperation of d-shells depends on many factors, such as the size of metal ion, oxidation number of metal ion, complex geometry, nature of metal ion, and the nature of the ligand. As the nature of the ligand is is easy to change and there are lots of ligands, effect of the nature of ligands on crystal field splitting parameter of a metal is selected as the question. As chromium(III) is common metal ion, easy to find and it forms d^3 complexes, which have spectrums relatively easy to interpret; the scope of the investigation is limited to chromium(III) complexes. So, the objective of this study to investigate the effect of the nature of ligand on the Octahedral Crystal Field Splitting Parameter(Δo) of chromium(III) complexes.

A variety of chromium (III) complexes with different ligands were synthesised; and characterized with UV-visible spectrometer. Then complexes' crystal field splitting parameters are calculated from the transition band with the longest wavelength. Also another method, involving Tanabe-Sugano diagrams, was used to calculate crystal field splitting parameters for comparison. It was found that there is no significant difference between the calculate crystal field splitting parameter values calculated from the transition band with the longest wavelength and values calculated from Tanabe-Sugano diagram.Overall, the crystal field splitting parameter values are found to be as 199442 J/mole for $Cr(acac)_3$, 258805 J/mole for $[Cr(en)_3]Cl_3$, 203020 J/mole for $[Cr(H_2O)_6](NO_3)_3$, 209766 J/mole for $K_3[Cr(ox)_3]$, 212761 J/mole for $K_3[Cr(NCS)_6]$. The order of the ligands in increasing order is found to be acac $<H_2O< C_2O_4^{2-}$ (ox)<NCS<en which matches mostly with the spectrochemical series, which shows the order as $C_2O_4^{2-}$(ox) $< H_2O < NCS^- <$ en.

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INTRODUCTION

The first time we did an experiment with copper sulphate pentahydrate($CuSO_4.5H_2O$) I was fascinated with it's blue color. The colour of copper in metal form is brownish, and it's colour in solution is blue. Although we know that reactants lose their properties when forming a product, I wondered why it is blue or not another colour.

Interested, I began researching this issue and found that the solutions of not only copper, but whole d-block(transition) elements are coloured. After my research, I found that the solutions of metals are called metal complexes, or coordination compounds. Metal complexes are combinations of metal ions and ligands. The ions of d-block metals have low energy unfilled d- and p- orbitals. These orbitals can accept a lone pair of electrons from some species, known as ligands, to form a dative bond between the ligand and the metal ion. As a source[1] indicates the colour difference in metal and solution form is resulted from splitting of d-orbitals while forming the bond. With octahedral ligands three orbitals are at low energy and two orbitals are at high energy. The difference in energy of these orbitals correspond to a frequency of light ($\Delta E = hf$), which is in the visible region of electromagnetic spectrum. Therefore, when white light passes through a metal complex, light of particular frequency is absorbed and an electron is promoted from a lower energy orbital to a higher energy orbital. From this issue, phenomenon called "complementary colors" is evolved. Complementary colors phenomenon states that if a compound absorbs light of one color, complement of absorbed color is seen. For example, in the case of most copper(II) compounds, red and yellow light are absorbed, so they look blue-green color. Also, the colours of gemstones are also explained with this phenomenon.

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[1] Green,John Damji,Sadru. Chemistry for use with the IBDP, IBID press,2001

After further research, I found that the energy difference between the upper (e_g) and lower(t_{2g}) energy levels is called Octahedral Crystal Field Splitting Parameter (Δo) or, 10 Dq.

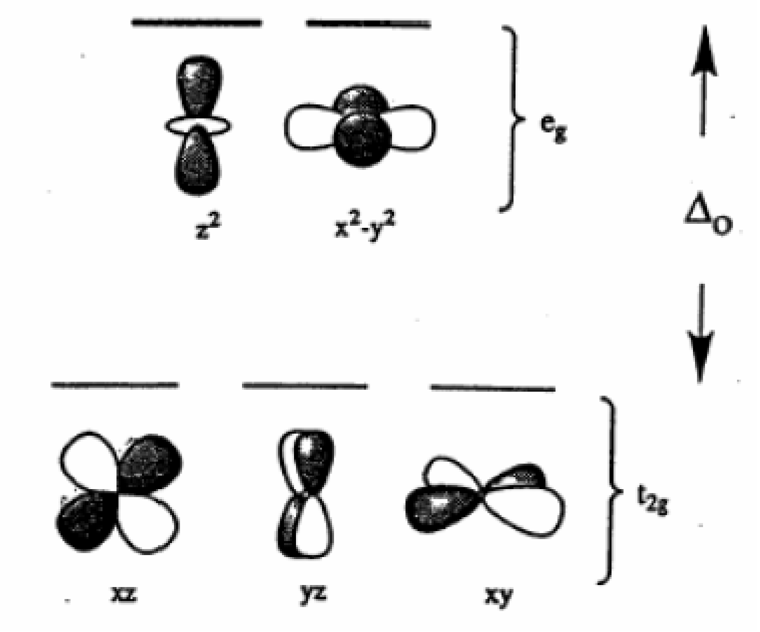

Fig.1: Splitting of energy levels of a octahedral complex

source

The degree of splitting of the *d* orbitals and hence the magnitude of Δo depends on several factors, including the charge on the metal, the size of the metal,and the nature of the ligand. I chose to investigate the effect of nature of ligand, because there are a lot of d-block metals and it is hard to plan an experiment with changing the nature of the metal and keeping the charge on the metal controlled. Also, I chose the chromium metal, because Chromium compounds (chromium(III) compounds, specifically) are *d*3 and their electronic spectral characteristics are reasonably easy to interpret. Consequently, this paper will focus on the research question “**What is the effect of the nature of ligand on the Octahedral Crystal Field Splitting Parameter(Δo) of chromium(III) complexes?”** and will discuss how the experiment done was planned and performed, as well as examining the results obtained by evaluating their validity and to attempt to analyse their possible consequences.

HYPOTHESIS

From a large number of studies, it is known that ligands can be arranged in a sequence according to their ability to cause d-orbital splitting. This series is known as the spectrochemical series[2]:

halides < OH^- < $C_2O_4^-$ < H_2O < NCS^- < py < NH_3 < en < phen < NO_2^- < CN^- < CO

The magnitude of Δo increases by a factor of about 2 as one moves from halide to CN– in the spectrochemical series. Carbon monoxide has the strongest ligand field of all the common ligands.

Therefore, it is hypothesised that, the the Δo of Tris(ethylenediamine)chromium(III) ($[Cr(en)_3]^{+3}$) will be larger than Hexa(thiocyanato)chromate(III) $[Cr(NCS)_6]^{-3}$ which will be larger than Tris(oxalato)chromate(III).

Also, as there are only 3 electrons present in d-shell in d3 complexes, the interaction fo the other two electron can be neglected. Therefore, Δo will be equal to the energy of the transition band with the longest wavelength

$$\Delta o = hc/\lambda$$

Where h is the plack's constant, c is the speed of light and λ is the wavelength of the transition band

From the spectrochemical series, it can be hypothesised that the UV spectogram of Tris(oxalato)chromate(III) will have a longer band than Hexa(thiocyanato)chromate(III), which will have a longer band than Tris(ethylenediamine)chromium(III). However, as the 2,4-pentanedionate is not a ligand in spectrochemical series, the UV spectrogram of Tris(2,4-

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[2] Zumdahl, Steven S. Chemical Principles Fifth Edition. Boston: Houghton Mifflin Company, 2005

pentanedionate)chromium(III) will be significantly different than other chromium(III) complexes.

METHOD DEVELOPMENT & PLANNING

Designing an appropiate method in order to support or reject the proposed hypothesis and answer the given research question brought various problems with it. One of the biggest problems was the lack of chemicals. I did not have the all chemicals to synthesise all complexes in the spectrochemical series, so I needed to synthesise just enough number of complexes to display the character of spectrochemical series. After, further research, I picked the ligands $C_2O_4^-$,H_2O and NCS^- in order to understand the change in **Δo** with consecutive ligands in spectrochemical series. Also, I picked ethylenediamine(en) to see the difference between 2 distant ligands in the spectrochemical series. Lastly, I picked 2,4-pentanedionate(acac), one of relavively the easiest complexes to synthesise in organometallic chemistry,because it is not in the spectrochemical series; allowing to see the difference between ligand in spectrochemical series and a ligand not in the spectrochemical series. Another reason for picking 2,4-pentanedionate is the it is one of relavively the easiest complexes to synthesise in organometallic chemistry.

Also, using the UV-visible spectrometer brought another problem, our school do not have a UV-visible spectrometer. After research I found a UV-visible spectrometer in Middle East Technical University Chemistry Department, I talked to proffessors in Chemistry department, and they kindly accepted to let me use their spectrometer.

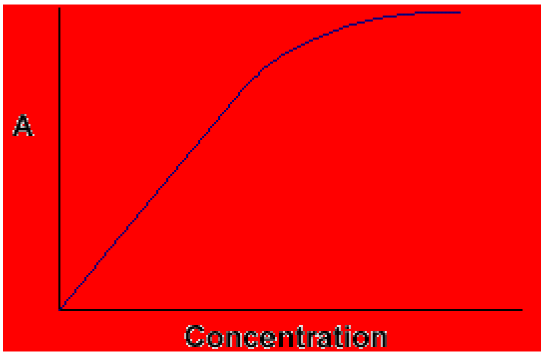
Now it is important to find synthesis procedures of selected complexes. After reseach, I found an extract from "Microscale Inorganic Chemistry: A Comprehensive Laboratory

Experience" by Szafran, Z.; Pike, R.M. and Singh, M.M., which includes all the procedures I needed.

Lastly, all necessary chemicals are provided at METU Chemistry Department. After that point Some Spectroscopy trials held with Potassium Tris(oxalato)chromate(III). Although only the λ_{max} values are needed, I observed that after a point, too much concentration of the analysed chemical can distort the spectrum. This can be explained with Beer-Lambert law. Beer-Lambert law states that

$$A=\varepsilon bc$$

Where A is absorbance(no units), ε is the molar absorbtivity coefficient(L mol^{-1} cm^{-1}), b is the path length of the sample(that is, the width of the cuvette)(cm) and c is the concentration of the compound in solution(M). As the formula shows that the absorbance increases linearly with the concentration, it is not the case. At higher values of c, deviations occur because of the interaction between molecules of compound.



In order to avoid this case, Spectroscopy trials were held with different concentrations of Potassium Tris(oxalato)chromate(III)

METHOD

Materials & Apparatus

Sizes and numbers are not indicated.....

Chromium chloride hexahydrate($CrCl_3 \cdot 6H_2O$) Erlenmeyer flask

Acetylacetone (2,4 Pentanedione)

Heater

Urea ($(NH_2)_2CO$)

Hirsch funnel

Filter paper

Distilled water

Ice

mossy zinc

methanol(CH_3OH)

toluene

ethylenediamine ($H_2N\text{-}CH_2CH_2\text{-}NH_2$)

reflux condenser

tweezers

evaporating dish

round bottom flask

Ether

potassium oxalate monohydrate($K_2C_2O_4 \cdot H_2O$)

oxalic acid dihydrate($H_2C_2O_4 \cdot 2H_2O$)

powdered potassium dichromate ($K_2Cr_2O_7$)

potassium thiocyanate (KSCN)

chrome alum ($KCr(SO_4)_2 \cdot 12H_2O$)

UV-visible spectrometer

2 ml Syringe

Preparation of Tris(2,4-pentanedionate)chromium(III).

Dissolve 260 mg of $CrCl_3 \bullet 6H_2O$ in 4.0 mL of distilled water within a small Erlenmeyer flask. Add 1 g of urea and 0,5 mL of acetylacetone. Heat the mixture to just below boiling with stirring for one hour. As the urea releases ammonia and the solution becomes basic, deep maroon crystals will begin to form. After one hour, cool the flask to room temperature. Collect the crystals by suction filtration. Wash the crystals with distilled water.

Preparation of Tris(ethylenediamine)chromium(III)

Add 100 mg of mossy zinc, 266 mg of $CrCl_3 \bullet 6H_2O$, and 1 mL of methanol to a 10 mL round bottom flask. In the hood, add 1 mL of ethylenediamine. Next place a reflux condenser on the flask, then reflux your reaction, with stirring, for one hour. Cool the solution to room temperature. Collect the yellow crystalline product by suction filtration using a Hirsch funnel. Remove any un-reacted zinc with tweezers. Wash the filtered product with 0.5 mL portions of 10% ethylenediamine in methanol until the washings are colorless. Follow this with a 0.5 mL rinse with ether. Allow the product to dry

Preparation of Potassium Tris(oxalato)chromate(III)

To a solution of 1,83 g potassium oxalate monohydrate and 4,67 g oxalic acid dihydrate in 70 ml water, 1,67 g powdered potassium dichromate is added in small portions with vigorous stirring. When the reaction has ended, the solution is evaporated nearly to 20% of its original volume and allows to crystallize in an ice water bath. Potassiun trioxalatochromate forms deep-green crystal. Collect the product by suction filtration, wash with 25 ml alcohol, then dry in oven

Preparation of Potassium Hexa(thiocyanato)chromate(III)

Make an aqueous solution of potassium thiocyanate, KSCN (2.5 g), chrome alum, $KCr(SO_4)_2\cdot 12H_2O$ (3.0 g) using distilled water (10 mL). Pour the solution into an evaporating dish and place on a steam bath. Evaporate to dryness, to obtain a mass of red crystals. Extract the solid, via suction filtration, using alcohol. The desired $K_3[Cr(NCS)_6]$, should dissolve very readily while K_2SO_4 remains as a residue. After evaporation of the filtered alcohol extract, collect the dark red-violet crystals

Spectroscopy of the Cr(III) Complexes.

Prepare aqueous solutions of tris(ethylenediamine)chromium(III) chloride , potassium tris(oxalato)chromate(III), potassium hexa(thiocyanato)chromate(III), and a toluene solution of tris(2,4-pentanedionate)chromium(III). Obtain the absorbance spectrum for each complex. Determine wavelength of peak which have maximum absorbance. Convert the wavelengths (which correspond to Δ_o) into wavenumbers using the following relationship:

$$\Delta\mathbf{o} = [hc/\lambda\ (\mathrm{nm})]$$

RESULTS

Synthesis of Complexes

Preparation of Tris(2,4-pentanedionate)chromium(III)

Trial	**Mass of $CrCl_3•6H_2O$ used (g)(±0,05)**	**Mass of urea used (g)(±0,05)**	**Volume of acetylacetone used (mL)(±0,05)**	**Mass of $Cr(acac)_3$ formed (g)(±0,05)**
1	0,76	1,01	1,00	0,82
2	0,77	1,01	1,00	0,92
3	0,76	1,00	1,00	0,85
4	0,75	1,02	1,00	0,92
5	0,76	1,00	1,00	0,96
6	0,76	1,00	1,00	0,90

Table ?

Preparation of Tris(ethylenediamine)chromium(III)

Trial	Mass of CrCl3•6H2O used (g)(±0,05)	Mass of urea used (g)(±0,05)	Volume of acetylacetone used (mL)(±0,05)	Mass of $Cr(acac)_3$ formed (g)(±0,05)
1	0,76	1,01	1,00	0,82
2	0,77	1,01	1,00	0,92
3	0,76	1,00	1,00	0,85
4	0,75	1,02	1,00	0,92
5	0,76	1,00	1,00	0,96
6	0,76	1,00	1,00	0,90

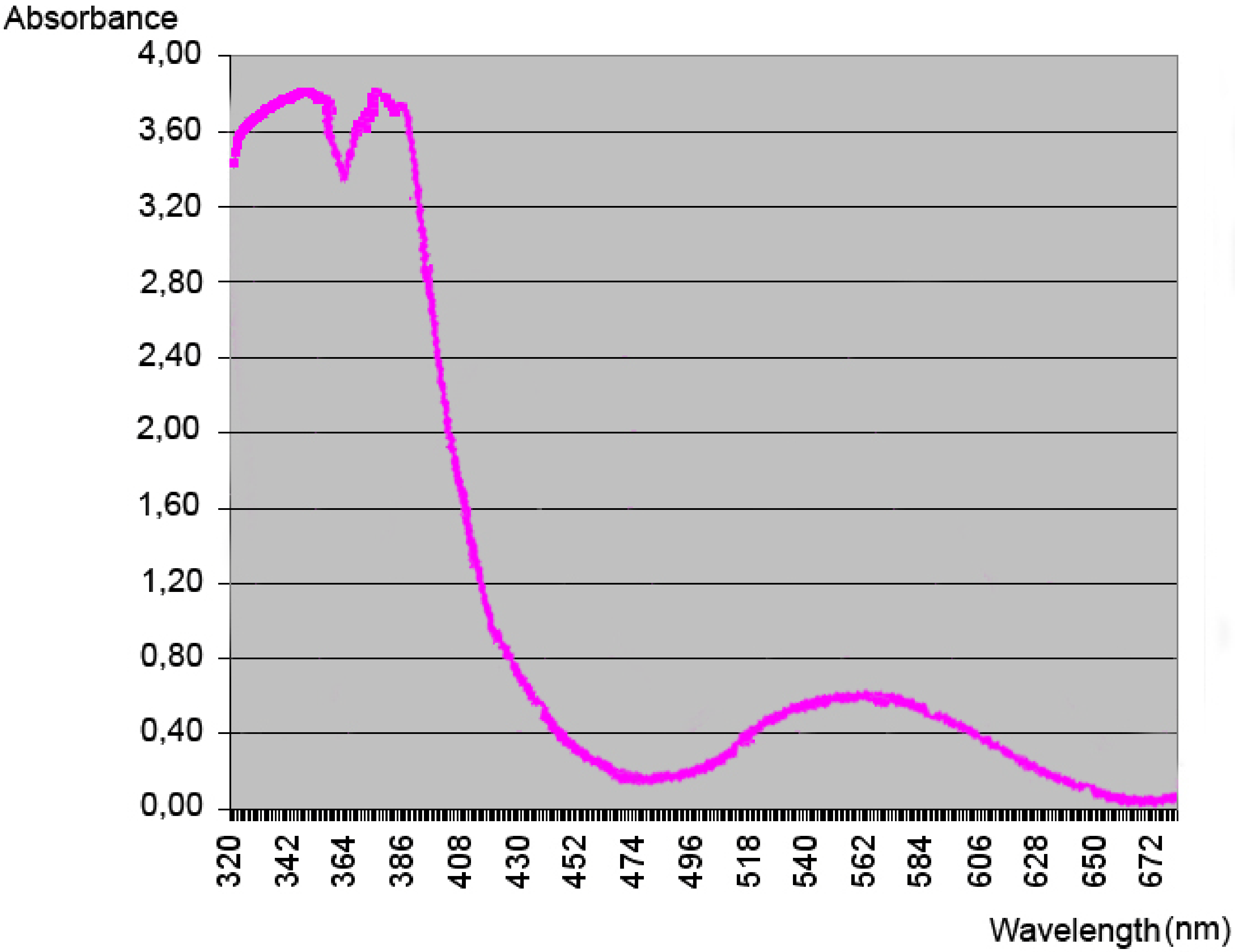
Preparation of Potassium Tris(oxalato)chromate(III)

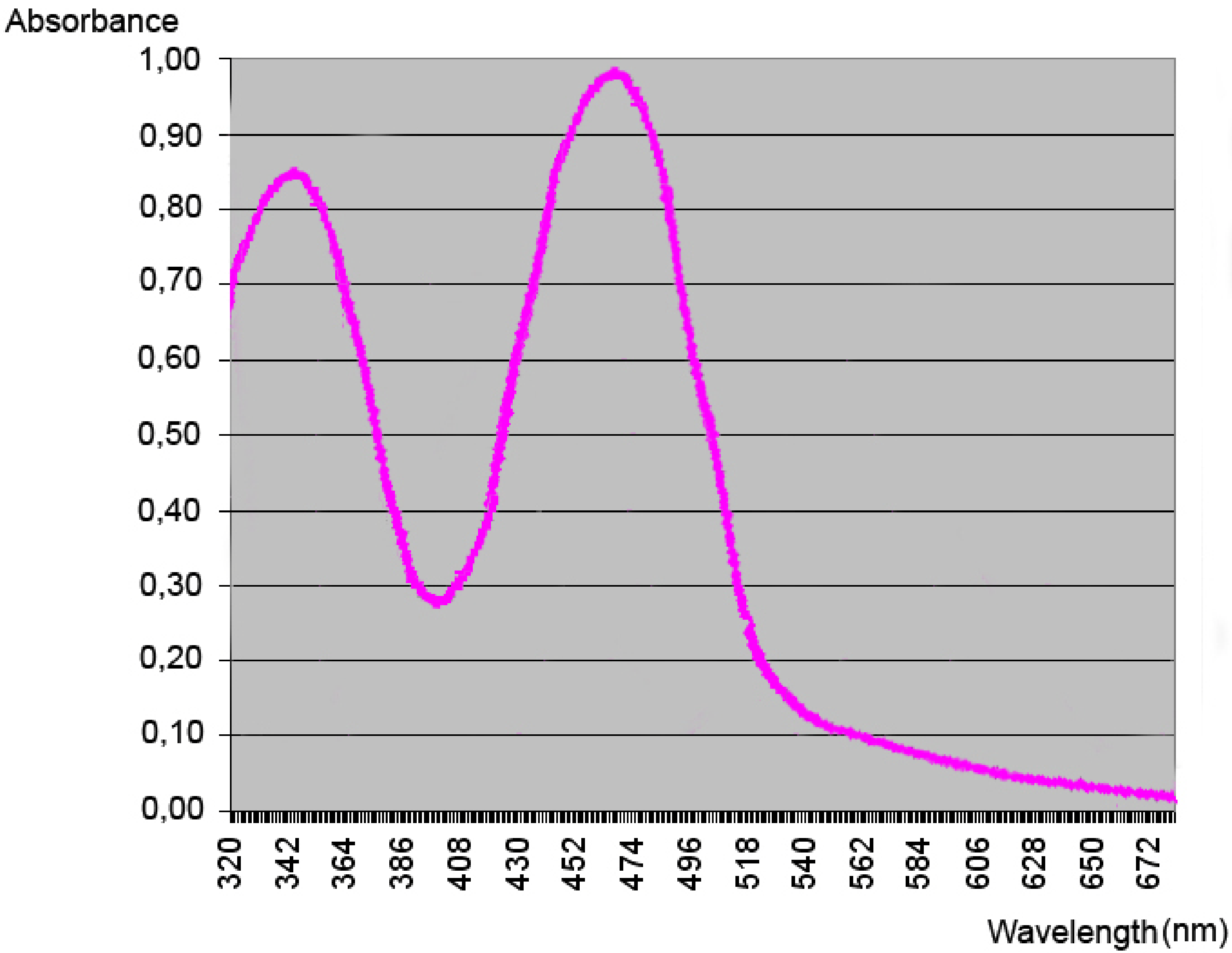
Trial	Mass of $K_2C_2O_4 \bullet H_2O$ used (g)(±0,05)	Mass of $K_2Cr_2O_7$ used (g)(±0,05)	Mass of $H_2C_2O_4 \bullet 2H_2O$ used (mL)(±0,05)	Mass of $K_3[Cr(C_2O_4)_3] \bullet 3H_2O$ formed (g)(±0,05)
1	1,83	1,67	4,67	4,21
2	1,83	1,67	4,67	4,30
3	1,83	1,67	4,67	4,25
4	1,83	1,67	4,67	4,29
5	1,83	1,67	4,67	4,30
6	1,83	1,67	4,67	4,25

Preparation of Potassium Hexa(thiocyanato)chromate(III)

Trial	Mass of $KCr(SO_4)_2 \cdot 12H_2O$ used (g)(±0,05)	Mass of KSCN used (g)(±0,05)	Mass of $K_3[Cr(NCS)_6]$ formed (g)(±0,05)
1	3,00	2,51	5,45
2	3,00	2,50	5,35
3	2,99	2,50	5,39
4	2,98	2,50	5,40
5	3,00	2,52	5,41
6	3,01	2,49	5,43

Spectrum of Cr^{+3} Complexes **(graph?)**




Absorbance
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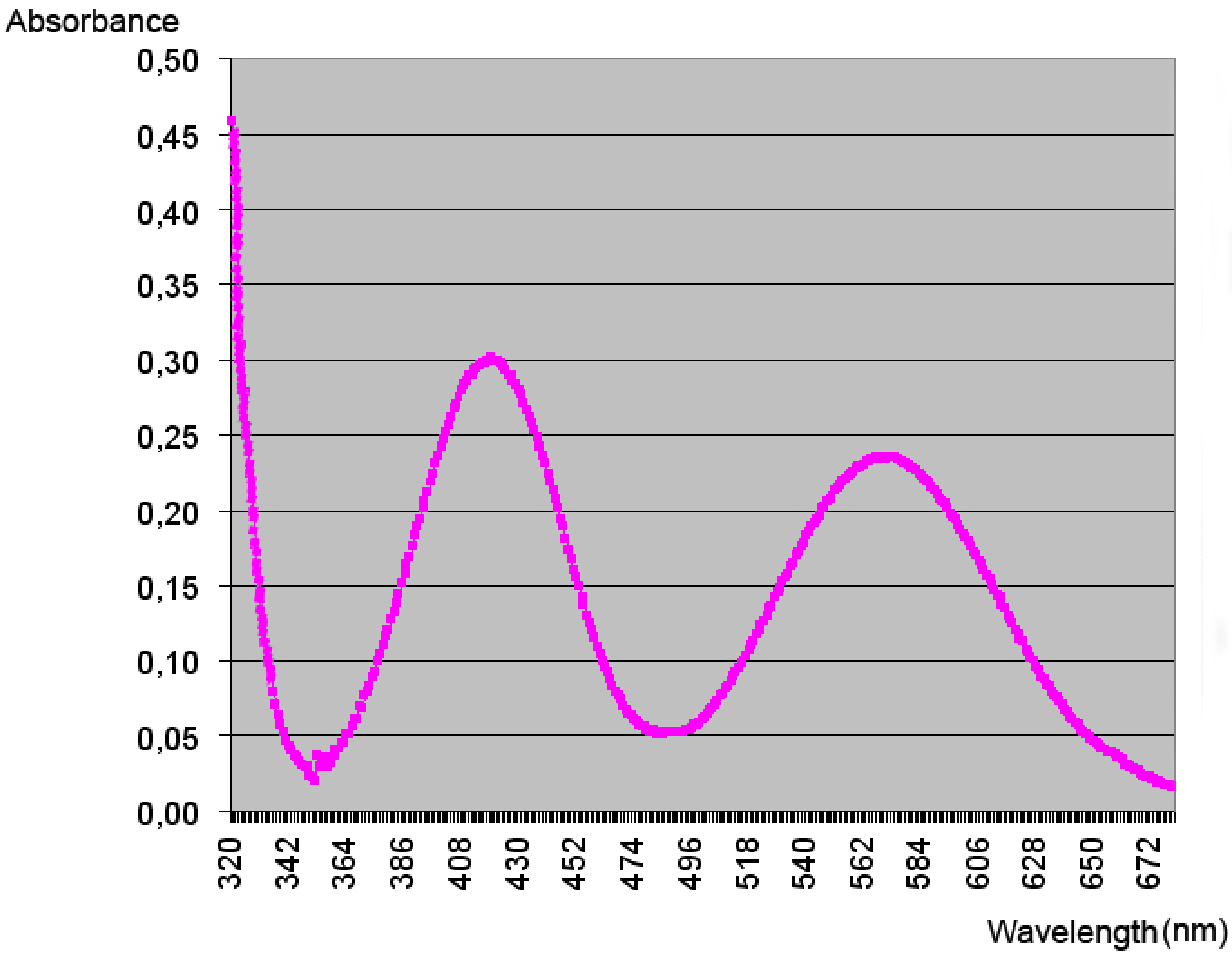
Wavelength (nm)


Absorbance
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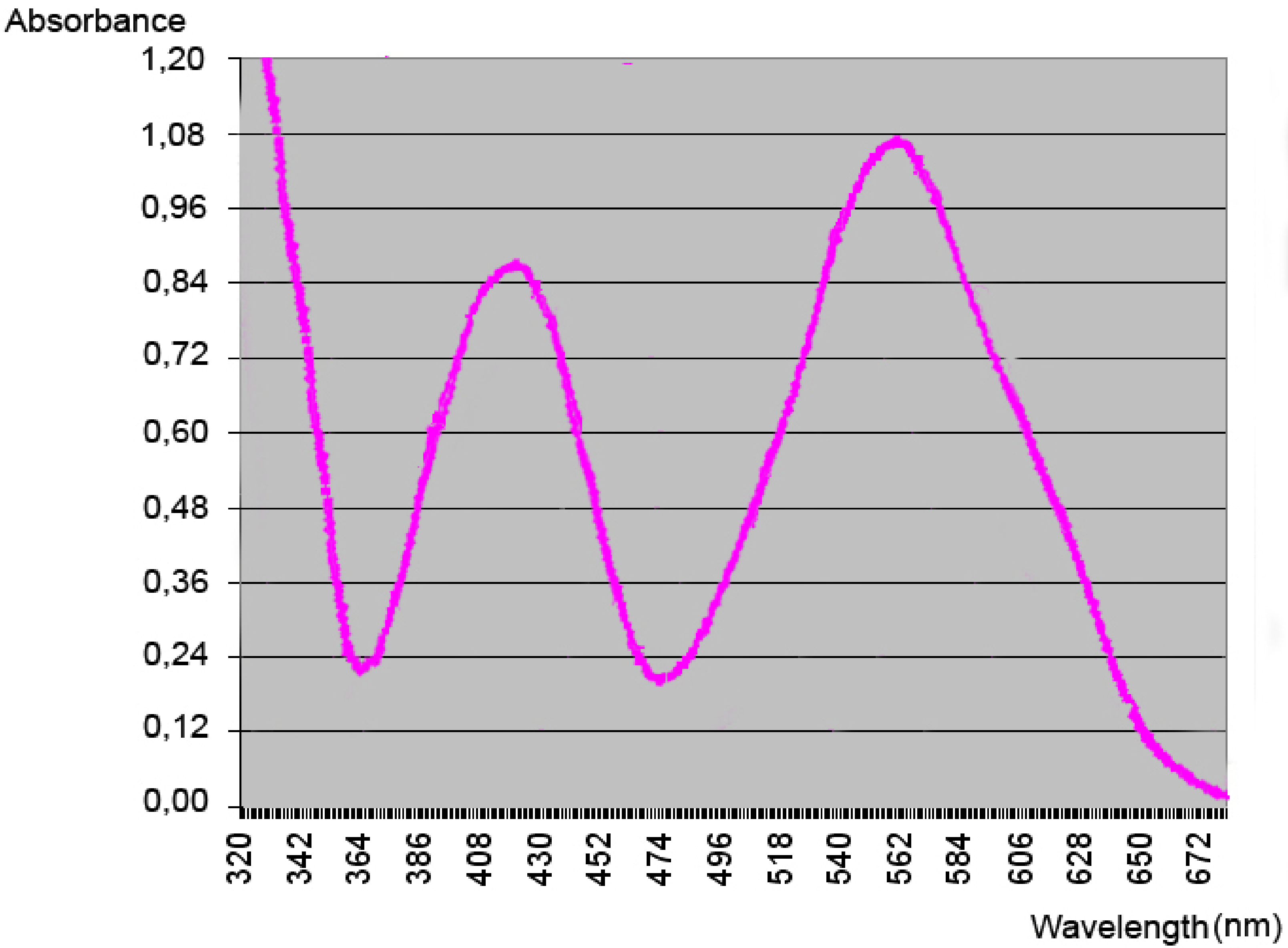
Wavelength (nm)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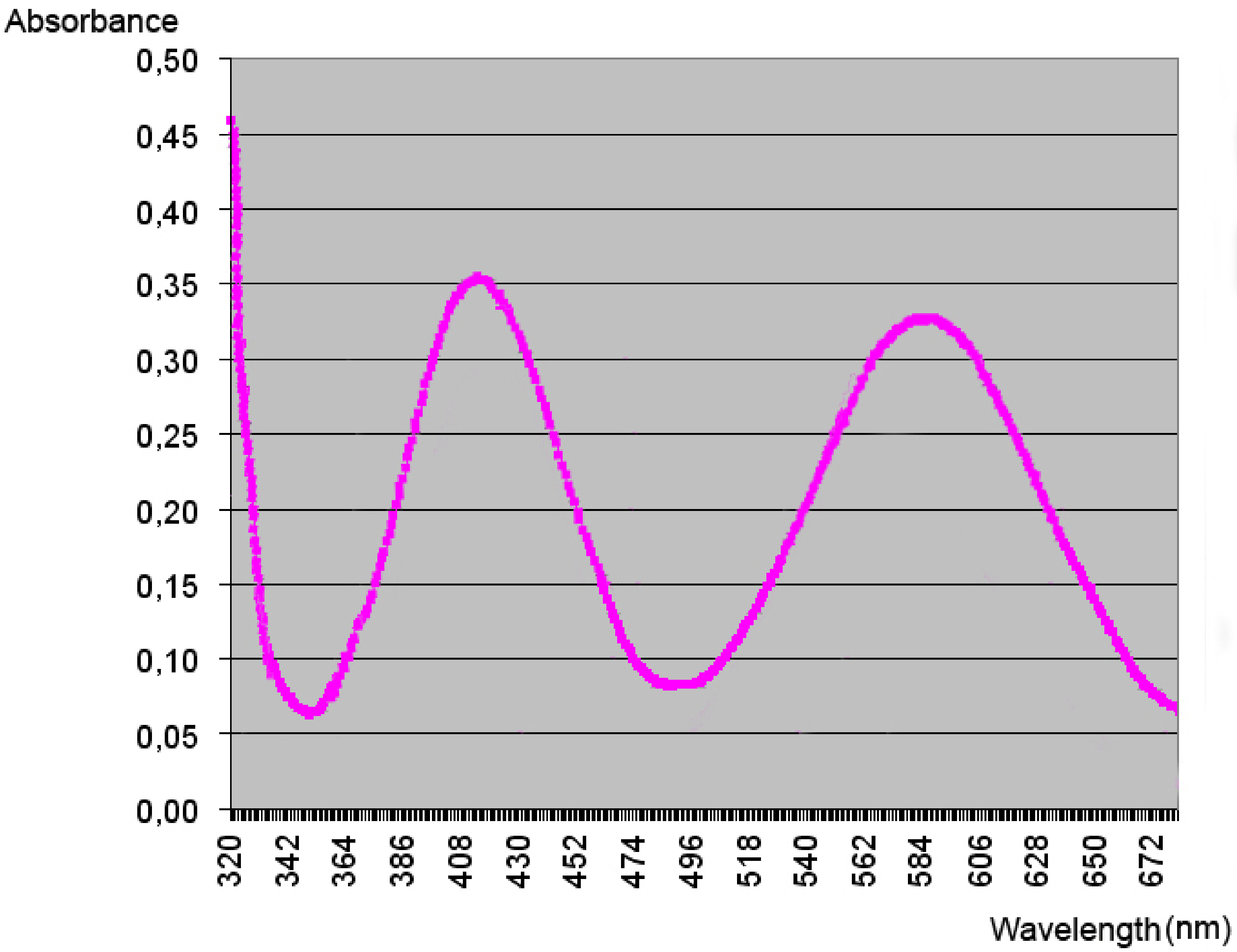
Wavelength (nm)


Absorbance
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Wavelength (nm)

DATA ANALYSIS

S

Spectroscopic Analysis

As for spectrochemical analysis, two analysis methods will be held. First method will be held is a simple and basic technique, which involves only the calculation of Δo by using the longest wavelength band. This method allows us to create a ranking between ligands, however, it does not yield accurate datas. As only the energy of the band with longest wavelength is assumed to have the energy of Δo, the additional interactions between d-electrons are neglected. This method is used for d1 complexes, however, as there are only 2 more electrons in a d3 complex, the interactions are at neglicible level(however, after d5 complexes, this interaction must be taken into account)

Complex	**λ_{max} (nm)(±1)**
$Cr(acac)_3$	560
$[Cr(en)_3]Cl_3$	459
$[Cr(H_2O)_6](NO_3)_3$	588
$K_3[Cr(ox)_3]$	570
$K_3[Cr(NCS)_6]$	562

The longest wavelength has the energy Δo,

$$\Delta o = E = hc / \lambda$$

For $Cr(acac)_3$,

$\Delta o = hc / (560 \times 10^{-9})$

$=(6,626 \times 10^{-34}\ Js \times 3,0 \times 10^{8}\ m/s) / (560 \times 10^{-9}\ m)$

$=3,55 \times 10^{-19}$ J for one molecule

$=3,55 \times 10^{-19} \times 6,02 \times 10^{23}$

=213688 J/mole

For $[Cr(en)_3]Cl_3$

Δo= hc / (459 x 10^{-9})

=(6,626x10^{-34} Js x 3,0x10^{8} m/s)/ (459 x 10^{-9} m)

=4,33x10^{-19} J for one molecule

=4,33x10^{-19} x 6,02x10^{23}

=260709 J/mole

For $[Cr(H_2O)_6](NO_3)_3$

Δo= hc / (588 x 10^{-9})

=(6,626x10^{-34} Js x 3,0x10^{8} m/s)/ (588 x 10^{-9} m)

=3,38x10^{-19} J for one molecule

=3,38x10^{-19} x 6,02x10^{23}

=203513 J/mole

For $K_3[Cr(ox)_3]$

Δo= hc / (570 x 10^{-9})

=(6,626x10^{-34} Js x 3,0x10^{8} m/s)/ (570 x 10^{-9} m)

=3,49x10^{-19} J for one molecule

=3,49x10^{-19} x 6,02x10^{23}

=209940 J/mole

For $K_3[Cr(NCS)_6]$

Δo= hc / (562 x 10^{-9})

=(6,626x10^{-34} Js x 3,0x10^{8} m/s)/ (562 x 10^{-9} m)

$=3{,}54\text{x}10^{-19}$ J for one molecule

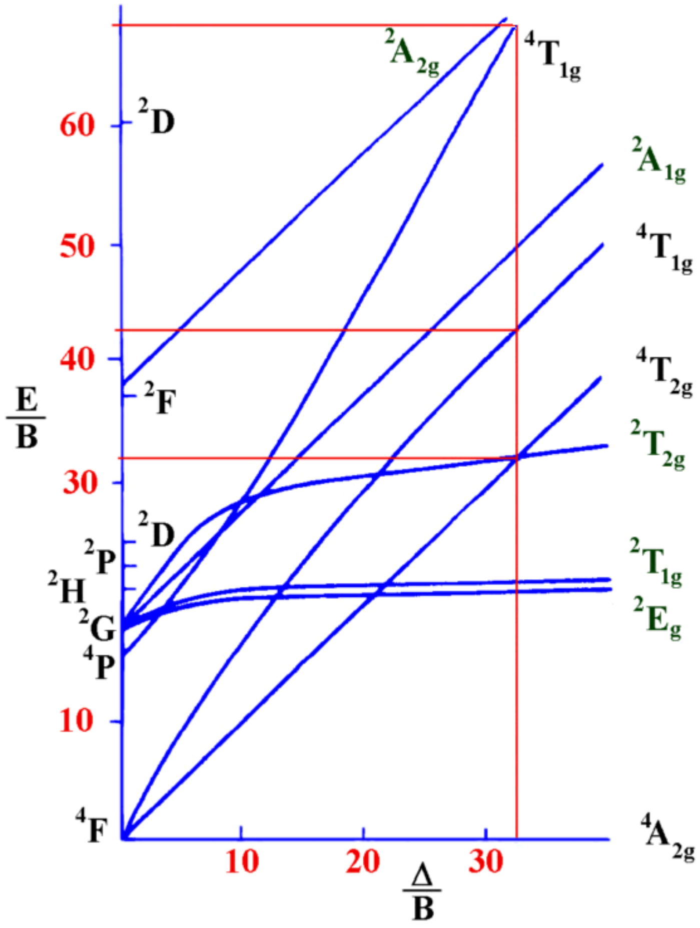
$=3{,}54\text{x}10^{-19}$ x $6{,}02\text{x}10^{23}$

=212928 J/mole

Complex	**Δo (J/mole) (± 368)**
$Cr(acac)_3$	213688
$[Cr(en)_3]Cl_3$	260709
$[Cr(H_2O)_6](NO_3)_3$	203513
$K_3[Cr(ox)_3]$	209940
$K_3[Cr(NCS)_6]$	212928

Spectroscopic Analysis Using Tanabe-Sugano Diagrams

The Tanabe-Sugano diagrams, are special cases of orgel diagrams, which helps us to calculate many variables of a complex accurately. As the Tanabe-Sugano diagrams involve the electronic interactions between the d-electrons, the calculations done using this diagrams are more accurate, However, as there are only 2 more electrons in a d3 complex, the interactions are neglicible, but there is small difference between the values calculated by the first method and the second method. In order to use the Tanabe Sugano Diagrams, the wavelengths are onverted into wavenumbers, then the ratio of v1 to v2 is found at the diagram.(v1 and v2 are the wavenumbers of first and second transition bands.There is a high energy(usually below 320nm) charge-transfer band, however these bands are not used in the calculations). From where the ratio falls on the diagram, E/B and Δo/B values are found. Racah parameter, B is found from the E/B ratio where E is the lowest transition energy in cm^{-1}. After B is found, Δo can be easily calculated from the Δo/B ratio



Example Calculation For Cr(acac)$_3$

Cr(acac)$_3$ has transition bands at 560 and 386 nm. Converting to wavenumbers, these values are 17857 and 25908 cm^{-1} respectively giving a v2/v1 ratio of 1,451. This ratio can be found at Δo/B= 21,160 and E/B=30,698. The band at 386 nm(25908 cm^{-1}) represents the $^4T_{1g} \leftarrow {}^4A_{2g}$(F) transition(lower energy) and the band at 560 nm(25908 cm^{-1}) represents the $^4T_{2g} \leftarrow {}^4A_{2g}$(F) transition(higher energy).

$$\frac{E}{B'}=30{,}698$$

$$E=25908\ cm^{-1}$$

$$B' = \frac{25908}{30{,}698} = 844{,}0\ cm^{-1}$$

$$\frac{\Delta o}{B'} = 21{,}160$$

$$\Delta o = 17859{,}0\ cm^{-1}$$

Converting to nanometers, this value becomes 600 nm.

$\Delta o = hc / (600 \times 10^{-9})$

$=(6{,}626 \times 10^{-34}\ Js \times 3{,}0 \times 10^{8}\ m/s) / (600 \times 10^{-9}\ m)$

$=3{,}31 \times 10^{-19}$ J for one molecule

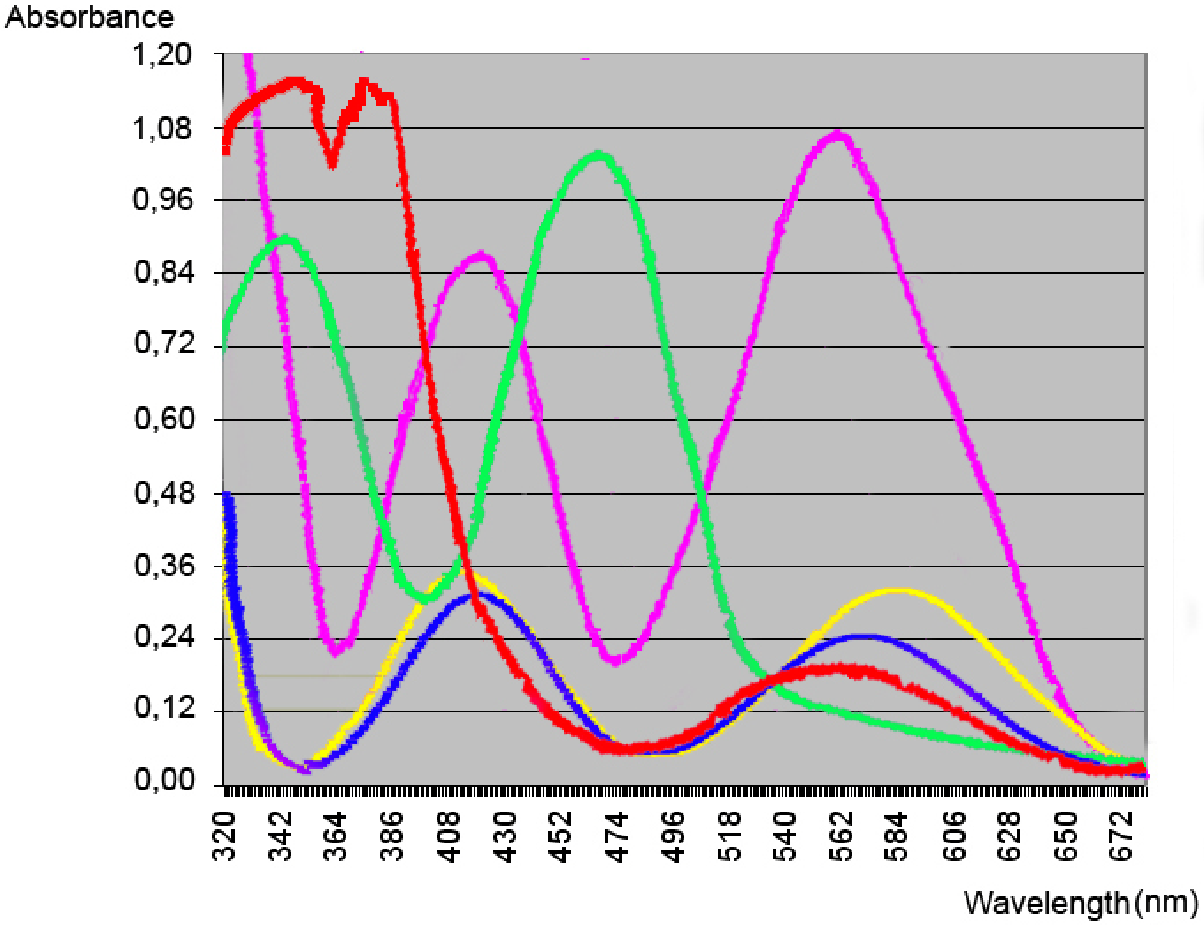
$=3{,}31 \times 10^{-19} \times 6{,}02 \times 10^{23}$ for one mole

=199442,6 J/mole

Complex	**V_1 (nm/cm^{-1})**	**V_2(nm/cm^{-1})**	**V_2/V_1**	**Δo/B**	**E/B**	**B(cm^{-1})**	**Δo(cm^{-1})**	**Δo (J/mole) (±362)**
$Cr(acac)_3$	560/17857	386/25908	1,45	21,160	30,698	844,0	17859,0	199442,6
$[Cr(en)_3]Cl_3$	462/21645	345/28986	1,34	30,860	41,321	701,5	21648,3	258805,5
$[Cr(H_2O)_6](NO_3)_3$	588/17006	416/24038	1,41	23,740	33,606	715,3	16981,0	203020,1
$K_3[Cr(ox)_3]$	570/17544	418/23923	1,36	28,300	38,587	620,0	17545,3	209766,7
$K_3[Cr(NCS)_6]$	562/17794	429/23310	1,31	34,380	45,033	517,6	17795,8	212761,6

Conclusion & Evaluation

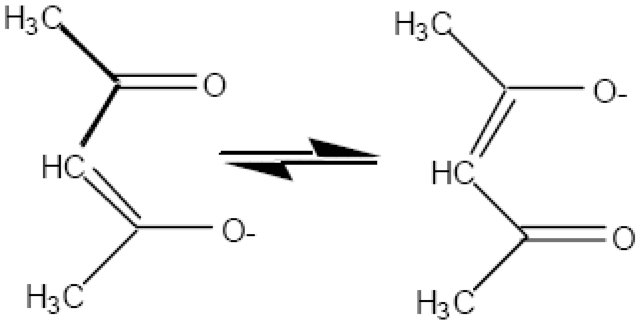
With nearly all assumptions in the hypothesis valid, this experiment shows that the order of ligands with ascending Δo is H_2O<ox<NCS<acac<en. This datas match with the spectrochemical series, however the Δo of oxalate ligand supposed to be smaller than aqua ligand. Also as hypothesised, the spectra of $Cr(acac)_3$ is significantly different than the other complexes.



Graph ? shows all spectrum of 5 Cr^{+3} complexes used in the experiment.

(red=$Cr(acac)_3$,green=$Cr(en)_3^{+3}$,Blue=$Cr(ox)_3^{-3}$,yellow=$Cr(H_2O)_6^{+3}$, pink=$Cr(NCS)_6^{-3}$)

As seen from graph, multiple maximas between 342-408 nm are only seen in $Cr(acac)_3$.Also the absorption values at maximas in other complexes are comparable, whereas there is a big difference between the maxima at 370 nm and the maxima at 560 nm. This can be resulted from the structure of acetylacetone. As acac$^-$ has resonance structure, which canbe seen in figure, might be the cause of the difference. Also, since the outer part of the complex is organic, the complex is hydrophobic, the spectroscopy was done solving the complex in toluene, which may affect the spectra.



Also, it is shown that there is a neglicible difference in Δo calculated with the longest wavelength band and Δo calculated with using Tanabe-Sugano diagrams.

Complex	**Δo (J/mole) (± 368)**	**Δo (J/mole) (±362)**	**Δ(Δo) (J/mole) (± 368)**	**Percentage difference (%)**
$Cr(acac)_3$	213688	199442	14246	7,14
$[Cr(en)_3]Cl_3$	260709	258805	1904	0,74
$[Cr(H_2O)_6](NO_3)_3$	203513	203020	493	0,24
$K_3[Cr(ox)_3]$	209940	209766	174	0,08
$K_3[Cr(NCS)_6]$	212928	212761	167	0,08

Therefore, the statement “for d3 complexes of Cr, the Δo equal to the energy of the transition band with the longest wavelength” is also valid

Several limitations have reduced the validity of hypothesis. First of all, when the ligand is changed, a lot of variables like field and molecular size also changes, therefore it is not certain that which variable of ligand affects the Δo of the complex. By definition, strong field ligands have higher Δo than weak field ligands, however it seems to be independant from molecular mass of ligands and the denticity

Also, there is the possibility that because of usage of excess reactants in synthesis $Cr(acac)_3$ and $[Cr(en)_3]Cl_3$ in order to increase the reaction speed, a stable $[CrCl_xL_y]^z$,is formed together with the desired complex (where L is the ligand and x,y are variable coefficients, and z is the oxidation number). This leads to impurity in the complex, and affecting the spectra. The expectional ordering of oxalate and aqua ligands can also explained with impurity.

To improve the experiment, trials with more ligands can be performed, to analyse the all ligands in the spectrochemical series, also in order to improve the purity, using excess reactants should be avoided, however, that will lead to lengthening of the synthesis time. Also, complexes should not be held for a long time before spectroscopy.

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