

Discovery-Based Approach to Identify Multiple Factors That Affect the Spin State of Coordination Complexes Using the Evans NMR Method

Masaki Uchida,* Candice H. Cortney, Karina Bustos, Elia Manzo, Emily Sauls, Jacob Bouchard, Risako Fukazawa, and Viswanathan V. Krishnan



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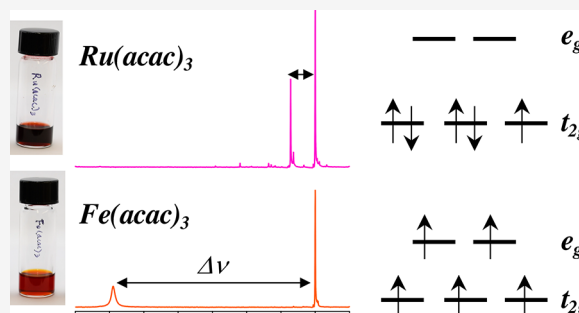
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ABSTRACT: Understanding the basics of d-electron configuration and the spin state of coordination complexes are essential elements of undergraduate inorganic chemistry. However, students in these courses find it difficult to conceptualize the ideas. Here, we have developed an undergraduate laboratory experiment that allows students to systematically evaluate the spin state of a set of coordination complexes composed of different ligands, metals, and the charge on a metal. Students assessed magnetic susceptibility and the number of unpaired electrons present on the metal centers of various complexes using the Evans method for NMR spectral data. They then identified the spin state of the complexes. Examining a series of complexes systematically leads students to discover three key factors that affect the spin state of coordination complexes: the type of ligand, the type of metal center, and the charge on the metal. A detailed description of the approach provided here can be implemented in inorganic and physical chemistry teaching laboratory settings.

KEYWORDS: Inorganic Chemistry, Laboratory Experiment, Evans Method, Coordination Complexes, Paramagnetic Substances, Magnetic Susceptibility, The Number of Unpaired Electrons, Spin State, NMR



INTRODUCTION

Electronic spin states of coordination complexes are a fundamental concept in an undergraduate inorganic chemistry course because they describe the physical and chemical properties of coordination complexes. Students typically learn that the d-electron configuration and the spin state of metal complexes can be explained by the crystal field theory (CFT) and the ligand field theory (LFT).^{1,2} However, it is often difficult for undergraduate students to grasp these concepts and ideas merely through lectures. By using experimental methods, students can relate molecular level changes to spectral changes, thus gaining a better understanding of the concepts as compared to traditional lecture-based exercises.^{3–5} Therefore, laboratory experiments associated with spin states are valuable components to actively engage students through hands-on experimentation to learn spin states and the factors that contribute to them. For example, several laboratory experiments have been reported, which adopted UV–vis spectroscopy characterization of various coordination complexes to generate a spectrochemical series and evaluate d-orbital splitting.^{3,4} These experiments are suitable to discuss the effect of ligands on d-orbital splitting, although the identification of the spin state of the complexes requires a

rigorous analysis of spectroscopic data using appropriate Tanabe–Sugano energy-level diagrams.³

Determining the number of unpaired electrons on the metal centers of coordination complexes through the magnetic susceptibility measurement could be another effective laboratory activity to compare the spin states of a series of complexes.⁵ As the magnetic susceptibility of transition metal complexes is closely related to the number of unpaired electrons, the number of unpaired electrons present on the metal center can be calculated from the magnetic susceptibility of the complexes. Although there are a few different methods to measure magnetic susceptibility,^{1,2,6} the use of the Evans method is a highly attractive analytical technique in an undergraduate laboratory course⁷ because nuclear magnetic resonance (NMR) spectroscopy is readily available for many teaching laboratories. Indeed, the Evans NMR method has been adopted into inorganic laboratory courses to analyze

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coordination complexes,^{8,9} most commonly metal acetylacetonates.⁶ In addition, for some complexes, the energy difference between the high-spin and the low-spin states is very small; thus their spin states can be changed by an external stimulus, such as heat or pressure.¹⁰ These are called spin-crossover complexes, and several laboratory experiments based on Fe(II) complexes have been reported for teaching laboratory courses.^{11–13} However, an experiment that evaluates only one or a few complexes with a single type of ligand can prove to be insufficient at fully communicating the concept of spin states. It is because of multiple factors, including the type of ligand, the type of metal center, and the charge on the metal, which all affect the d-electron configuration and the spin state of the complexes.

Here, we developed a laboratory experiment that is designed to lead students to discover those three key factors mentioned above (Figure S1). First, students examined the magnetic susceptibility of various metal acetylacetonate complexes with different transition metal centers and determined the number of unpaired electrons of the complexes. Next, they investigated various metal aqua and metal cyanide complexes. Finally, they analyzed and compared the spin states of the investigated complexes with different ligands, metals, and charge on the metals. Through the comprehensive analysis of the obtained results, students identified various factors that affected the spin state of the complexes and acquired a deeper insight into coordination chemistry.

Learning Outcomes for Students

The experimental activity reported here would be suited for an undergraduate inorganic chemistry and physical chemistry teaching laboratory course. The learning outcomes students would obtain through this experiment and the postexperiment discussion activities are as follows:

- (1) Acquire basic experimental skills and safety precautions to synthesize metal coordination complexes.
- (2) Identify the oxidation state and d-electron configurations of the metal centers.
- (3) Explain the geometry of coordination complexes and their coordination numbers.
- (4) Describe the difference between the high- and low-spin states and draw d-orbital splitting diagrams of coordination complexes.
- (5) Analyze what factors contribute to the spin state of coordination complexes.
- (6) Interpret NMR data to assess magnetic susceptibility and the number of unpaired electrons of measured complexes.
- (7) Describe the experimental approach to analyze the spin state of coordination complexes.

■ EXPERIMENTAL SECTION

Synthesis and NMR Measurement of Metal Acetylacetonate Complexes

In the first part of the laboratory experiment, students analyzed magnetic susceptibilities and the number of unpaired electrons of various metal acetylacetonate (acac) complexes (Cr(acac)₃, Mn(acac)₃, Fe(acac)₃, Co(acac)₃, and Ru(acac)₃) (Figure S2a). Among these complexes, Mn(acac)₃ was synthesized⁶ by students, thereby acquiring basic experimental skills and safety precautions to synthesize metal coordination complexes. Because of time constraints, other complexes were purchased

from Fisher Scientific, Tokyo Chemical Industry, or Sigma-Aldrich. The ¹H NMR peak shift due to the presence of a paramagnetic compound was examined by using two chemicals, tetramethylsilane (TMS) and CHCl₃, as internal reference compounds to monitor the ¹H NMR peak shift due to the presence of a paramagnetic complex. The detailed procedures of the sample preparation and NMR measurements are given in the Supporting Information.

Preparation and NMR Measurement of Metal Aqua and Metal Cyanide Complexes

In the second part of this experiment, students prepared and analyzed various metal aqua complexes ([Fe(III)(H₂O)₆]³⁺, [Co(II)(H₂O)₆]²⁺, and [Co(III)(H₂O)₆]³⁺) and metal cyanide (CN) complexes ([Fe(II)(CN)₆]⁴⁻, Fe(III)(CN)₆³⁻, and Co(III)(CN)₆³⁻) (Figure S2b and c). Solutions of [Co(II)(H₂O)₆]²⁺, [Co(III)(H₂O)₆]³⁺, and [Fe(III)(H₂O)₆]³⁺ were prepared by adapting previous reports with minor modifications.^{3,14,15} Two NMR reference compounds, sodium 3-(trimethylsilyl)-1-propanesulfonate (DSS) and H₂O, were used to monitor the ¹H NMR peak shift. The detailed procedures of the sample preparation and NMR measurement are given in the Supporting Information.

NMR Measurement

The magnetic susceptibility of the various coordination complexes was determined by the Evans NMR method. An NMR tube with a coaxial insert (Chemglass, C-NISCCI-B) was used for the measurement. Approximately 150 μL of a sample solution containing each coordination complex and 600 μL of the reference solution without the coordination complex were added into the coaxial inner tube and the outer tube, respectively (Figure S3). NMR spectra of sample solutions were collected with a 300 MHz NMR spectrometer (Bruker Fourier 300 spectrometer; Billerica, MA). The detailed procedure is available in the Supporting Information.

Data Analysis

Molar magnetic susceptibility of a dissolved coordination complex, χ_M (in units of cm³/mol), can be determined by the Evans method with the following equation:^{6,16,17}

$$\chi_M = \frac{\Delta\nu}{S_f\nu_0} \times \frac{1000}{c} \quad (1)$$

where $\Delta\nu$ is the observed peak shift of a reference compound in hertz between those in the outer tube and in the coaxial inner tube containing a coordination complex as a solute (here, the downfield peak shift due to a paramagnetic complex is considered as positive $\Delta\nu$), ν_0 is the frequency of the NMR spectrometer in hertz, and c is the molar concentration of solute (in units of mol/L). S_f in eq 1 is the shape factor of the magnet used in the NMR spectrometer.^{6,16,18–20} In the case of conventional NMR spectrometers with permanent magnets or electromagnets, which create a magnetic field perpendicular to the long axis of the sample tube, S_f becomes $\frac{-2\pi}{3}$, while modern high-field NMR spectrometers equipped with superconducting solenoids, which generate a magnetic field parallel to the long axis, correspond to $S_f = \frac{4\pi}{3}$.^{16,21} In this experiment, a 300 MHz NMR with superconducting solenoids was used for the measurements; thus $S_f = \frac{4\pi}{3}$ was applied for the data analysis.

Measured magnetic susceptibility of a compound χ_M is the sum of paramagnetic contributions, χ_M^{para} , and diamagnetic contributions, χ_M^{dia} , with the following equation:^{16,22}

$$\chi_M = \chi_M^{\text{para}} + \chi_M^{\text{dia}} \quad (2)$$

Paramagnetic contribution arises from unpaired electrons on a metal center of a coordination complex, whereas the diamagnetic component arises from the sum of paired electrons of the inner core of the metal and the ligands coordinated to the metal. In this study, diamagnetic correction factors of the transition metals and various ligands were obtained from previous literature (Table S1).^{6,23} The effective magnetic moment, μ_{eff} , can be obtained from χ_M^{para} with the following equation:^{1,2,6,9}

$$\mu_{\text{eff}} = \sqrt{8\chi_M^{\text{para}} T} \quad (3)$$

where T is the temperature of the measurement in kelvin. Assuming that only unpaired electrons in a coordination complex contribute to the magnetic moment, the number of unpaired electrons on the metal center of a coordination complex, n , can be determined with the following equation:^{1,2,6,9}

$$\mu_{\text{eff}} = \sqrt{n(n+2)} \quad (4)$$

It should be noted that for some metal complexes such as the second- and third-row transition metal complexes, the orbital angular momentum of electrons can also contribute to the magnetic properties of the complexes.^{2,6} Nevertheless, the μ_{eff} provides a useful approximation to determine the number of unpaired electrons and works well for the $\text{Ru}(\text{acac})_3$ in this experiment.^{2,5,6}

HAZARDS

Proper personal protective equipment (PPE), including gloves, goggles, and lab coat, should be used at all times. Reactions should be performed in a well-ventilated area. Students should understand laboratory safety and how to handle hazardous materials. A copy of the SDS for each hazardous chemical should be available, and potential hazards should be discussed before performing any experiment. Hydrogen peroxide, nitric acid, and perchloric acid are highly corrosive and can cause irritation to the eyes and mucous membranes. In case of contact, rinse the affected area with water for at least 15 min. Chloroform and its deuterated counterpart are very volatile and can be dangerous if inhaled. TMS is highly flammable and should not be used near an open flame. When $\text{Mn}(\text{acac})_3$ is synthesized, acetylacetonate should be added slowly to avoid the reaction overflowing its container. Chemicals should never be poured down the drain and should be appropriately disposed of according to appropriate laboratory practices set by each institution. Additional notes for waste collection are available as the instructor's notes in the [Supporting Information](#).

RESULTS AND DISCUSSION

Metal Acetylacetonate Complexes

Representative ^1H NMR spectra of the sample solutions containing various metal acetylacetonate complexes are shown in Figure 1a. For these complexes, deuterated chloroform was used as the solvent, and TMS and chloroform were used as reference compounds to determine $\Delta\nu$ (Table 1a). The ^1H

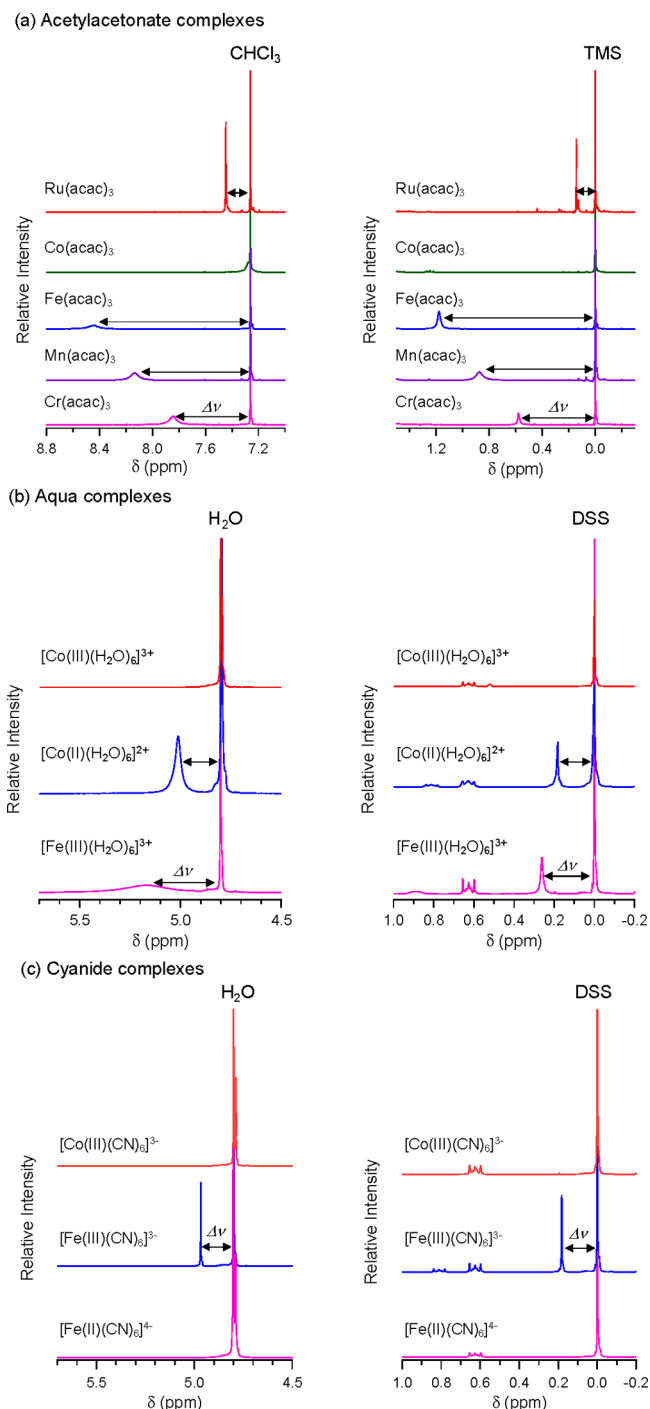


Figure 1. ^1H NMR spectra of reference compounds with various coordination complexes: (a) acetylacetonate complexes, (b) aqua complexes, and (c) cyanide complexes. TMS and DSS in the coaxial outer tube appear at 0 ppm. CHCl_3 and H_2O in the outer tube appear around 7.26 and 4.80 ppm, respectively. These compounds in the inner tubes appear downfield in the presence of paramagnetic compounds. Small triplet peaks around 0.6 ppm in the DSS graphs are attributed to the hydrogen of CH_2 in DSS.

NMR peaks attributed to TMS and chloroform in pure solvent (the outer tube) appeared at 0.00 and 7.26 ppm, respectively. The ^1H peaks of these two standard compounds arising from the coaxial inner tube, in which approximately 20 mM of a metal acetylacetonate complex was dissolved, appeared downfield with broader peak widths, except the sample containing

Table 1. Summary of Representative Students' Data Including Magnetic Susceptibilities and the Number of Unpaired Electrons Calculated from the Observed Peak Shifts of Reference Compounds Due to the Presence of Various Coordination Complexes: (a) Acetylacetonate Complexes, (b) Aqua Complexes, and (c) Cyanide Complexes

(a) Acetylacetonate Complexes							
compd	conc (mM)	TMS			chloroform		
		Δ (ppm)	χ_M^{para} ($\text{cm}^3 \text{mol}^{-1}$)	n	Δ (ppm)	χ_M^{para} ($\text{cm}^3 \text{mol}^{-1}$)	n
Cr(acac) ₃	22.1	0.58	6.36×10^{-3}	3.02	0.59	6.47×10^{-3}	3.05
Mn(acac) ₃	21.1	0.88	1.01×10^{-2}	3.99	0.87	1.00×10^{-2}	3.97
Fe(acac) ₃	19.54	1.18	1.46×10^{-2}	4.98	1.18	1.46×10^{-2}	4.98
Co(acac) ₃	20.5	0	0	0	0	0	0
Ru(acac) ₃	20.1	0.14	1.83×10^{-3}	1.32	0.19	2.43×10^{-3}	1.60
(b) Aqua Complexes							
compd	conc (mM)	DSS			H ₂ O		
		Δ (ppm)	χ_M^{para} ($\text{cm}^3 \text{mol}^{-1}$)	n	Δ (ppm)	χ_M^{para} ($\text{cm}^3 \text{mol}^{-1}$)	n
[Fe(H ₂ O) ₆] ³⁺	5.0	0.26	1.26×10^{-2}	4.57	0.36	1.74×10^{-2}	5.53
[Co(H ₂ O) ₆] ²⁺	5.7	0.18	7.59×10^{-3}	3.37	0.21	8.87×10^{-3}	3.70
[Co(H ₂ O) ₆] ³⁺	5.4	0	0	0	0	0	0
(c) Cyanide Complexes							
compd	conc (mM)	DSS			H ₂ O		
		Δ (ppm)	χ_M^{para} ($\text{cm}^3 \text{mol}^{-1}$)	n	Δ (ppm)	χ_M^{para} ($\text{cm}^3 \text{mol}^{-1}$)	n
[Fe(CN) ₆] ⁴⁻	21.5	0	0	0	0	0	0
[Fe(CN) ₆] ³⁻	21.9	0.18	2.08×10^{-3}	1.44	0.17	1.91×10^{-3}	1.36
[Co(CN) ₆] ³⁻	20.2	0	0	0	0	0	0

Co(acac)₃ complex, which did not show a detectable peak shift (Figure 1a). This result indicates that Cr(acac)₃, Mn(acac)₃, Fe(acac)₃, and Ru(acac)₃ are paramagnetic compounds, whereas Co(acac)₃ is a diamagnetic compound. The degree of the peak shift increased in the order of Ru(acac)₃, Cr(acac)₃, Mn(acac)₃, and Fe(acac)₃ under the same concentration of complexes. In addition, the peak shift of Ru(acac)₃ was significantly less than that of Fe(acac)₃ despite the fact that both complexes are d⁵ metal complexes with identical ligands. As is discussed later, it is because the Fe(acac)₃ complex takes a high-spin state, whereas the Ru(acac)₃ complex takes a low-spin state. Magnetic susceptibility and the number of unpaired electrons of each compound were calculated as described in the Data Analysis and as summarized in Table 1a (in the Supporting Information, a student handout table is provided where students can summarize the results, including the d-orbital splitting diagrams). It should be noted that the $\Delta\nu$ values of the two reference compounds, TMS and chloroform, in the same sample are nearly identical. Measuring the two reference compounds simultaneously gave the students confidence in their results. The number of unpaired electrons of Cr(acac)₃, Mn(acac)₃, Fe(acac)₃, Co(acac)₃, and Ru(acac)₃ complexes calculated from the NMR results (the average value obtained from TMS and chloroform) were 3.0, 4.0, 5.0, 0, and 1.5, respectively. This supports the theoretical values of 3, 4, 5, 0, and 1, respectively. From this result, students could identify that Mn(acac)₃ and Fe(acac)₃ complexes take a high-spin state (i.e., the electron configuration of $t_{2g}^3e_g^1$ and $t_{2g}^3e_g^2$, respectively) rather than the low-spin state (i.e., $t_{2g}^4e_g^0$ and $t_{2g}^5e_g^0$, respectively). However, Co(acac)₃ and Ru(acac)₃ complexes take a low-spin state (i.e., the electron configuration of $t_{2g}^6e_g^0$ and $t_{2g}^5e_g^0$, respectively), although the coordinated ligands are identical in the four complexes. From this result, students discovered that the type of the metal center affects the d-electron configuration and spin state of the complexes.

Because Cr(acac)₃ is the d³ metal complex, there is no distinction between high-spin and low-spin states, and the complex takes only one electron configuration (i.e., $t_{2g}^3e_g^0$).

Metal Aqua and Metal Cyanide Complexes

The sample solutions containing various metal aqua complexes and metal cyanide complexes were also analyzed with ¹H NMR spectroscopy (Figure 1b and c). D₂O was used as the solvent for these complexes, and DSS and H₂O were supplemented as reference compounds to determine $\Delta\nu$ (Table 1b and c). The number of unpaired electrons of [Fe(III)(H₂O)₆]³⁺, [Co(II)(H₂O)₆]²⁺, and [Co(III)(H₂O)₆]³⁺ estimated from the NMR measurements were 5, 3, and 0, respectively. This result indicates that [Co(II)(H₂O)₆]²⁺ is a high-spin compound, whereas [Co(III)(H₂O)₆]³⁺ is a low-spin compound, demonstrating that the charge on the metal center is another factor that affects the spin state of complexes. Similarly, the number of unpaired electrons of [Fe(II)(CN)₆]⁴⁻, [Fe(III)(CN)₆]³⁻, and [Co(III)(CN)₆]³⁻ was estimated as 0, 1, and 0, respectively, indicating that all three complexes take the low-spin state. By comparing the spin state of Fe(acac)₃, [Fe(III)(H₂O)₆]³⁺, and [Fe(III)(CN)₆]³⁻, students recognized that the type of ligand is another factor that affects the spin state of the complexes; cyanide ligand induces a larger d-orbital splitting than do acetylacetonate and aqua ligands and thus results in taking the low-spin state.

Assessment of Learning Outcomes

This laboratory experiment was initially developed in the semester of Spring 2020 through the collaboration of undergraduate students and faculty members. The experimental procedure was implemented in an inorganic chemistry teaching laboratory course in the Spring 2022 (13 students) and Spring 2023 (15 students) semesters in person as one of the laboratory projects. Students conducted this experiment and analyzed the data in groups of three or four students per group. They completed this experiment in three weeks (two

separate three-hour laboratory sections per week), followed by one additional section for discussion (Table S2). To assess the learning outcomes in the four categories (Table 2), quizzes

Table 2. Learning Objectives Assessed by Quiz Questions

question category	evaluating point for each category
1	identify the oxidation state of metal center and its d electron counts
2	identify coordination number and geometry of coordination complex
3	distinguish between high-spin state and low-spin state and draw the d-orbital splitting diagram of coordination compounds
4	discuss factors that affect the spin state of coordination compounds

were given to the students pre- and postlaboratory in the semester of Spring 2023. The results of the assessment are shown in Figure 2. Although all students in the lab course had

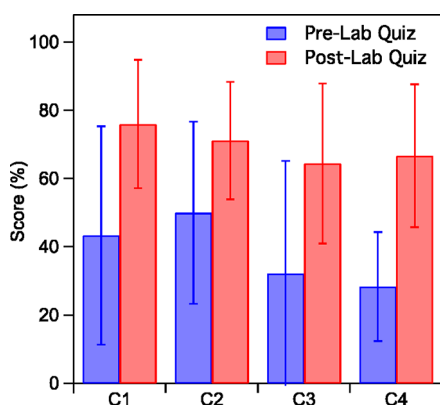


Figure 2. Comparison of the results of the pre- and postlaboratory quizzes that aim to evaluate students' achievement in the four categories of learning objectives.

taken an inorganic chemistry lecture course and learned about coordination chemistry before enrolling into the lab course, most of the students had relatively weak knowledge of coordination complexes in all four categories before conducting this experiment. The quizzes to evaluate the achievement of each learning objective significantly improved after this experiment, indicating that this experiment is effective in advancing students' understanding of the important concepts in coordination chemistry.

The students' feedback also strongly supported that this experiment serves as a promising teaching laboratory project for deepening students' understanding of d-electron configuration and the spin state of coordination complexes. One student commented in a free-writing section of a postlab survey form that "My understanding of d-orbital splitting and spin states has grown by synthesizing and studying complexes and then determining the number of unpaired electrons. This has further solidified the concept of d-orbital splitting and spin states because the link between unpaired electrons and paramagnetic properties was tangible and much more apparent than reading about it in literature." Another comment included, "Changing a couple of factors and seeing what happens really helped me see not only the link between complexes and their properties but also how a chemist

approaches a problem and tweaks factors in order to understand a concept."

CONCLUSIONS

This laboratory experiment was developed to demonstrate the effect of three key factors on the spin state of coordination complexes, the type of ligand, the type of metal center, and the charge on the metal, and was successfully implemented in an inorganic chemistry teaching laboratory course. Students investigated the magnetic susceptibility of various coordination complexes using the Evans method, calculated the number of unpaired electrons, and identified the spin state of the complex. Through a systematic approach, students discovered that all three factors contribute to the d-electron configuration and spin states of the coordination complexes. The insights students acquire through discovery-based laboratory learning enhanced their understanding of some key concepts of coordination chemistry.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at <https://pubs.acs.org/doi/10.1021/acs.jchemed.3c00738>.

Experimental procedure, supplementary data and figures, and instructor's notes (PDF, DOCX)
 Postlab quiz (PDF, DOCX)
 Postlab answer key (PDF, DOCX)
 Handout table for students (PDF, DOCX)

AUTHOR INFORMATION

Corresponding Author

Masaki Uchida – Department of Chemistry and Biochemistry, California State University, Fresno, California 93740, United States; orcid.org/0000-0003-0710-8834; Phone: (559) 278-2237; Email: muchida@mail.fresnostate.edu; Fax: (559) 278-4402

Authors

Candice H. Cortney – Department of Chemistry and Biochemistry, California State University, Fresno, California 93740, United States

Karina Bustos – Department of Chemistry and Biochemistry, California State University, Fresno, California 93740, United States

Elia Manzo – Department of Chemistry and Biochemistry, California State University, Fresno, California 93740, United States

Emily Sauls – Department of Chemistry and Biochemistry, California State University, Fresno, California 93740, United States

Jacob Bouchard – Department of Chemistry and Biochemistry, California State University, Fresno, California 93740, United States

Risako Fukazawa – Department of Chemistry and Biochemistry, California State University, Fresno, California 93740, United States

Viswanathan V. Krishnan – Department of Chemistry and Biochemistry, California State University, Fresno, California 93740, United States; orcid.org/0000-0002-0726-950X

Complete contact information is available at: <https://pubs.acs.org/10.1021/acs.jchemed.3c00738>

Notes

The authors declare no competing financial interest.

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