



## **Stability Constant of Metal Ligand and Complex**

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### **Abstract**

This paper explores the stability constant of metal-ligand complexes, a key parameter in coordination chemistry that defines the affinity between a metal ion and its ligand. By examining methods of determination, including potentiometric, spectrophotometric, and conductometric techniques, the study emphasizes the accuracy and applicability of different experimental approaches. Results demonstrate that factors such as metal ion charge, ligand denticity, solvent polarity, and temperature significantly affect stability. The analysis reveals that chelating ligands enhance complex stability due to the chelate effect, while environmental conditions further modify equilibrium constants. The findings confirm that stability constants play a pivotal role in advancing applications in bioinorganic chemistry, drug design, catalysis, and environmental remediation.

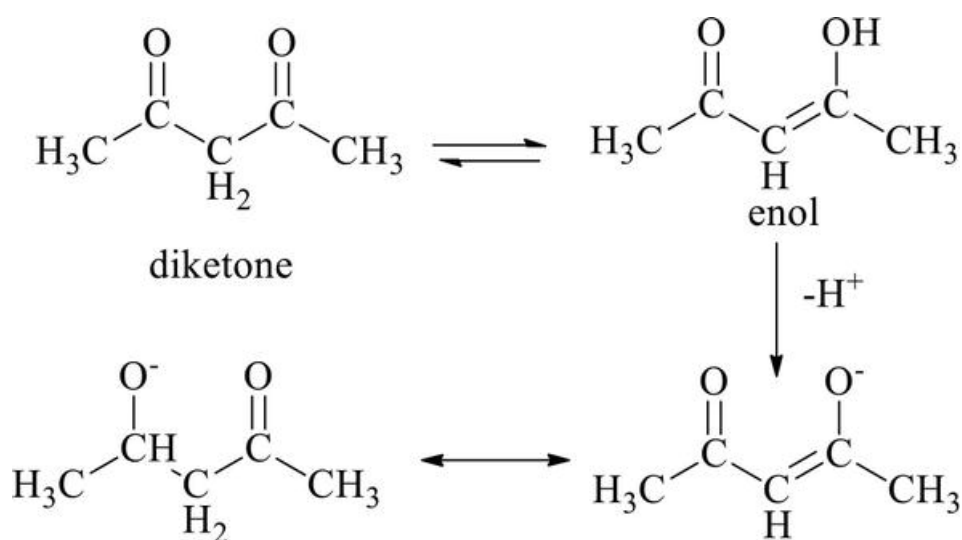
**Keywords:** Stability constant, metal-ligand complex, coordination chemistry, chelate effect, potentiometric methods, spectrophotometry, bioinorganic chemistry, catalysis.

### **Introduction**

Metal-ligand complexes play a central role in coordination chemistry, bioinorganic chemistry, and industrial applications such as catalysis, drug design, and environmental remediation. The stability constant, often referred to as the formation constant ( $K_f$ ), is a quantitative measure of the affinity between a metal ion and its ligand. A higher stability constant indicates stronger binding, which directly affects the reactivity, selectivity, and biological significance of the complex. Understanding stability constants provides insight into chemical equilibria, predicts reaction pathways, and guides the design of new metal-based compounds for pharmaceuticals, sensors, and industrial catalysts (Singh et al. 2019). This study focuses on the stability constant of metal-ligand complexes, discussing experimental methods of determination, factors influencing stability, and their practical implications. One of the most critical parameters used to describe the strength and stability of these interactions is the stability constant (also known as the formation constant,  $K_f$ ). This

constant provides a quantitative measure of the affinity between a metal ion and a ligand, reflecting the equilibrium position of the complexation reaction.

The study of stability constants is essential because it helps in predicting the feasibility of complex formation, understanding reaction mechanisms, and explaining selective binding in both natural and synthetic systems. For instance, stability constants determine how effectively a ligand can bind to toxic heavy metals for environmental remediation or to biologically essential metals such as  $\text{Fe}^{2+}$ ,  $\text{Cu}^{2+}$ , or  $\text{Zn}^{2+}$  in living organisms. Moreover, stability data guide the rational design of drugs, catalysts, and advanced materials, ensuring that the desired interactions are achieved under specific conditions (Gutten and Rulisek, 2013). Over the decades, various experimental and theoretical methods have been developed to measure and interpret stability constants, including potentiometry, spectrophotometry, calorimetry, and computational modeling. Each approach provides unique insights into the thermodynamic and kinetic aspects of metal-ligand interactions. Given the growing importance of metal complexes in medicine, environmental chemistry, and materials science, revisiting the concept of stability constants remains crucial for both fundamental understanding and practical application.



### Rationale of the study

The stability constant of metal-ligand complexes is crucial to predicting chemical behavior in both natural and synthetic systems. For example, in biological systems, metal ions such as  $\text{Fe}^{2+}$ ,  $\text{Cu}^{2+}$ , and  $\text{Zn}^{2+}$  form stable complexes with biomolecules, influencing processes like oxygen transport, enzyme catalysis, and electron transfer. Similarly, in environmental

chemistry, the stability of heavy metal complexes with ligands determines their toxicity, mobility, and removal efficiency. Despite the extensive study of metal-ligand complexes, understanding the underlying principles that govern their stability remains vital for advancing applications in medicine, catalysis, and materials science. Hence, this study is significant in providing a comprehensive overview of the stability constant and its importance in multiple domains (Okoye et al. 2019).

Ligands	Metal : Ligand	$\lambda_{\max}$ (nm)	M : L	Stability constant (log $\beta$ )
<b>Trimethoprim</b>	Cu (II) TMP	650	1 : 2	11.27
	Fe (III) TMP	660	1 : 2	10.99
	Zn (II) TMP	255	1 : 2	10.00
	Ni (II) TMP	645	1 : 2	10.75
	Co (II) TMP	650	1 : 2	8.92
<b>Sulphadiazine</b>	Cu (II) SAZ	640	1 : 2	6.31
	Ni (II) SAZ	652	1 : 2	5.43
	Fe(II)SAZ	410	1 : 2	5.93
	Co (II) SAZ	540	1 : 2	5.29
	Zn (II) SAZ	274	1 : 2	3.92
<b>Sulphadimidine</b>	Cu (II) SAD	635	1 : 2	5.43
	Ni (II) SAD	675	1 : 2	5.03
	Fe (II) SAD	415	1 : 2	5.19
	Co (II) SAD	535	1 : 2	4.62
	Zn (II) SAD	282	1 : 2	4.20

### Determination of stability constant

The stability constants of metal ions ( $\text{Co}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Fe}^{3+}$ ) with ligand (SAD, SAZ and TMP) were determined spectrophotometrically using the modified procedure of Hilderbrand and Benesi<sup>13</sup> as described by Lamsa *et al.*<sup>14</sup> & Rose and Drago<sup>15</sup>. A series of seven solutions were prepared with a constant concentration of metal ion  $[\text{M}_0]$  and variable ligand,  $[\text{L}_0]$  concentration at pH 7.4 with ionic strength (0.1M  $\text{KNO}_3$ ). The reaction mixture

In medicinal chemistry, drugs such as cisplatin rely on stability and ligand exchange processes to exert anticancer effects, while chelation therapy for heavy-metal poisoning is designed around ligands that form highly stable complexes with toxic ions. In environmental contexts, understanding stability constants helps predict the mobility of heavy metals in soil and water, as well as their potential bioavailability and toxicity.

Ligand	lgK <sub>c</sub>				
	Ni <sup>2+</sup>	Zn <sup>2+</sup>	Cd <sup>2+</sup>	Cu <sup>2+</sup>	Pb <sup>2+</sup>
NH <sub>3</sub>	2.8	2.37	2.65	4.25	
Glutathione (RS <sup>1-</sup> )	4.0	5.0	6.16		
Imidazole (=N)	3.0	2.52	2.8		
Acetate (O <sup>1-</sup> )	0.8	0.7	1.2		
Glycine		5.52	4.8	8.62	5.47
Oxalate		4.68	4.0	6.19	4.0
OH		4.4	4.6	6.3	6.2
Carbonate		4.8	4.0	6.77	6.2
Humic acids (pH8)		5.3	5.0	5.0	5.3-8
Surface particles (pH8)		-3.6	-3.7	-1.8	-1.7

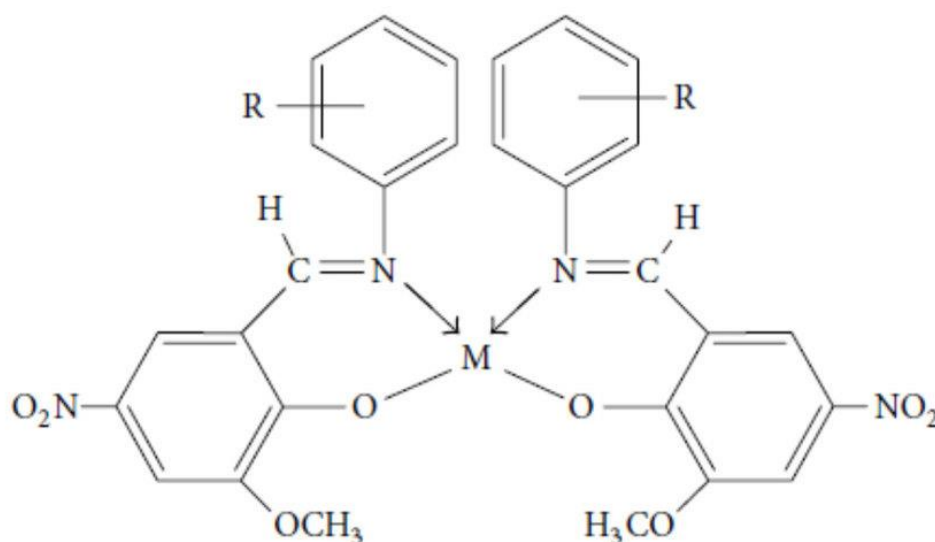
Despite their wide-ranging applications, stability constants are influenced by numerous factors including the charge density of the metal ion, the denticity and basicity of the ligand, solvent polarity, ionic strength, and temperature. Thus, a systematic study of stability constants provides a framework for optimizing conditions in laboratory experiments and industrial processes. This research is rationalized by the need to consolidate the theoretical foundations and experimental methods associated with stability constant determination, while also highlighting its practical significance. By exploring both intrinsic (metal and ligand properties) and extrinsic (environmental and experimental) factors, the study aims to bridge

the gap between classical coordination chemistry and its applications in modern scientific fields. Ultimately, a deeper understanding of stability constants will contribute to the advancement of bioinorganic chemistry, drug discovery, catalysis, and environmental sustainability.

## **Literature Review**

### **Fundamentals of Metal-Ligand Complexes**

Metal-ligand complexes are formed when a central metal ion binds with one or more ligands through coordinate covalent bonds, where the ligand donates electron pairs to the metal. The geometry and stability of these complexes are influenced by the coordination number of the metal, ligand denticity, and the electronic structure of the metal ion. Complexes may be classified as simple (monodentate ligands) or chelating (multidentate ligands), with chelating agents typically providing greater stability due to the chelate effect. Understanding the fundamentals of metal-ligand interactions is essential for explaining phenomena such as electronic transitions, magnetic properties, and reactivity. These foundational concepts serve as the basis for exploring the thermodynamic stability and equilibrium properties of complexes, which are quantified by stability constants (Fanourakis and Phipps, 2023).

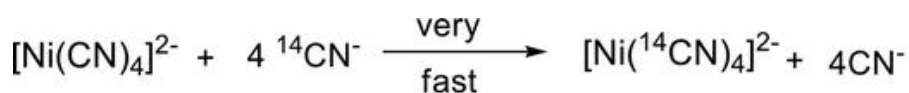


Metal-ligand complexes are formed when a central metal ion binds with surrounding molecules or ions known as ligands through coordinate covalent bonds, where the ligand donates an electron pair to the metal. The number of donor atoms attached to the metal, known as the coordination number, determines the geometry of the complex, which can be octahedral, tetrahedral, or square planar depending on the metal's electronic configuration.

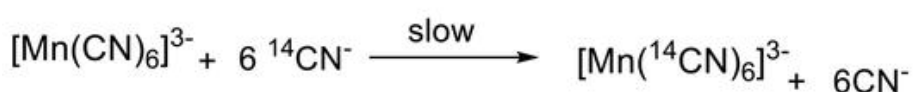
Ligands are broadly classified as monodentate, which bind through a single donor atom such as  $\text{NH}_3$  or  $\text{Cl}^-$ , and polydentate (chelating agents), which bind through multiple donor atoms, forming ring-like structures that enhance stability through the chelate effect. The stability of these complexes is quantitatively expressed by stability constants, also known as formation constants ( $K_f$ ), which define the equilibrium position of the reaction between metal ions and ligands. The magnitude of these constants reflects the affinity between the metal and the ligand, with higher values indicating stronger binding (Mareliati et al. 2022). Such interactions are not only fundamental to coordination chemistry but also play key roles in biological systems, as seen in the binding of oxygen to the iron center of hemoglobin, in analytical chemistry through EDTA titrations, and in industrial catalysis where stable complexes govern reactivity and selectivity.

### **Methods of Determining Stability Constants**

Several experimental and theoretical approaches have been developed to measure stability constants accurately. Potentiometric titration is one of the most common techniques, involving pH measurements to determine proton displacement during complex formation. Spectrophotometric methods utilize UV-Visible absorption changes upon complexation, allowing direct correlation between absorbance and equilibrium concentrations.



$$t_{1/2} = 30 \text{sec}$$



$$t_{1/2} = 1 \text{hr}$$



$$t_{1/2} = 24 \text{days}$$

Conductometric methods measure changes in solution conductivity as complexes form, while calorimetric studies provide insights into enthalpic contributions (Gulcin and Alwasel, 2022). In recent years, computational modeling and software-based fitting tools have enhanced the



precision of stability constant determination by simulating complex equilibria. Each method has its advantages and limitations, and the choice depends on the nature of the metal-ligand system under study.

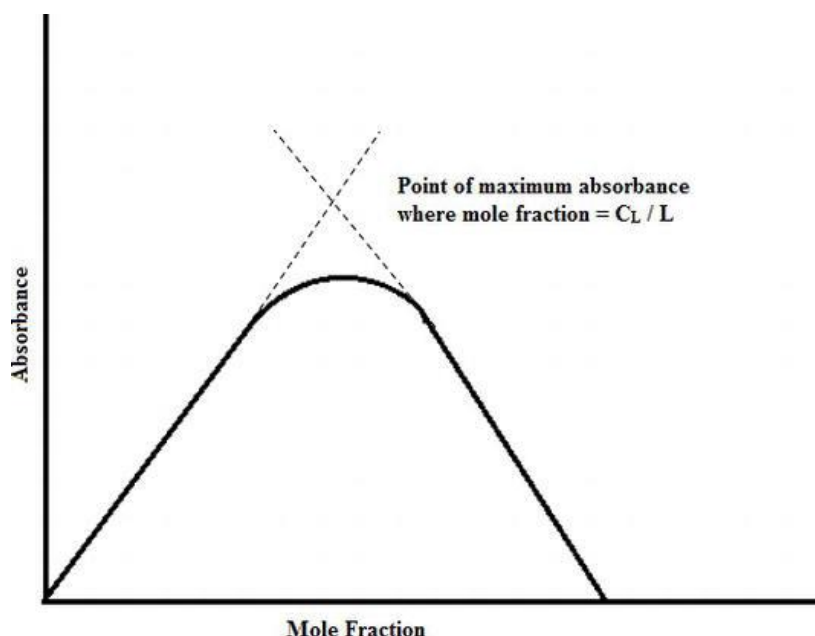
The determination of stability constants is essential for understanding the thermodynamic properties of metal-ligand complexes, and several experimental methods have been developed for this purpose. One of the most common approaches is potentiometric titration, where changes in pH are monitored as a ligand is titrated against a metal ion solution, allowing equilibrium constants to be calculated from the titration curve. Spectrophotometric methods are also widely employed, taking advantage of the fact that many complexes exhibit characteristic absorption spectra; by monitoring absorbance changes at specific wavelengths and applying the Beer–Lambert law, stability constants can be derived. Similarly, fluorimetric techniques are used when complexes display fluorescence properties, providing high sensitivity for dilute solutions. Conductometric methods rely on measuring the changes in electrical conductivity as complexation alters the ionic mobility in solution. In addition, calorimetric studies measure the heat evolved or absorbed during complex formation, giving insight into both enthalpy and equilibrium constants (Harvey et al. 2022). Advanced techniques such as NMR spectroscopy and mass spectrometry are increasingly used to provide structural as well as quantitative information on complex stability, particularly for biologically relevant ligands. Computational methods, including molecular modeling and density functional theory (DFT) calculations, also complement experimental approaches by predicting stability constants and providing deeper insight into metal-ligand interactions. The choice of method typically depends on the solubility, stability, and spectroscopic properties of the system under study, with potentiometry and spectrophotometry being the most widely adopted in coordination chemistry.

### **Factors Influencing Stability Constants**

The magnitude of a stability constant is governed by both intrinsic and extrinsic factors. Intrinsic factors include the nature of the metal ion—its charge density, ionic radius, and electronic configuration—as well as the properties of the ligand such as basicity, denticity, and steric hindrance. Chelating ligands generally form more stable complexes compared to monodentate ligands due to entropy gain (chelate effect) (Tang et al. 2019). Extrinsic factors include solvent polarity, ionic strength, and temperature, all of which can alter the

equilibrium position. For instance, polar solvents stabilize charged species, increasing the apparent stability of complexes, while higher temperatures may shift equilibria due to changes in enthalpy and entropy. Understanding these factors is critical for predicting and tailoring the behavior of complexes in different environments.

The stability constant of a metal-ligand complex is governed by a variety of chemical and environmental factors that determine the strength and nature of the interaction between the metal ion and the ligand. One of the primary influences is the nature of the metal ion, including its charge, ionic radius, and electronic configuration; for instance, metal ions with higher charges and smaller radii tend to form stronger complexes due to greater electrostatic attraction.



The hard and soft acid-base (HSAB) principle also plays a critical role, as hard acids like alkali metals preferentially bind to hard bases such as oxygen donors, while soft acids like transition metals prefer soft bases such as sulfur or nitrogen donors (Ardean et al. 2021). The structure and denticity of the ligand significantly affect stability, with multidentate ligands forming more stable complexes through the chelate effect, which arises from the entropic advantage of multiple binding sites. Additionally, the steric hindrance introduced by bulky substituents can either enhance or weaken stability depending on how they influence binding geometry. Solvent effects are another key factor, since polarity, dielectric constant, and solvation of both the free ions and the complex can alter equilibrium positions. Changes in pH influence protonation states of ligands, thereby affecting their ability to coordinate with



metal ions. Furthermore, temperature and ionic strength can shift equilibrium by modifying enthalpic and entropic contributions to binding. In biological systems, the presence of competing ligands, macromolecular scaffolds, and microenvironmental conditions (such as in enzymes or metalloproteins) also strongly influence complex stability (Tsuboyama et al. 2023). Thus, stability constants are not absolute values but context-dependent, reflecting a delicate balance between intrinsic chemical properties and external environmental factors.

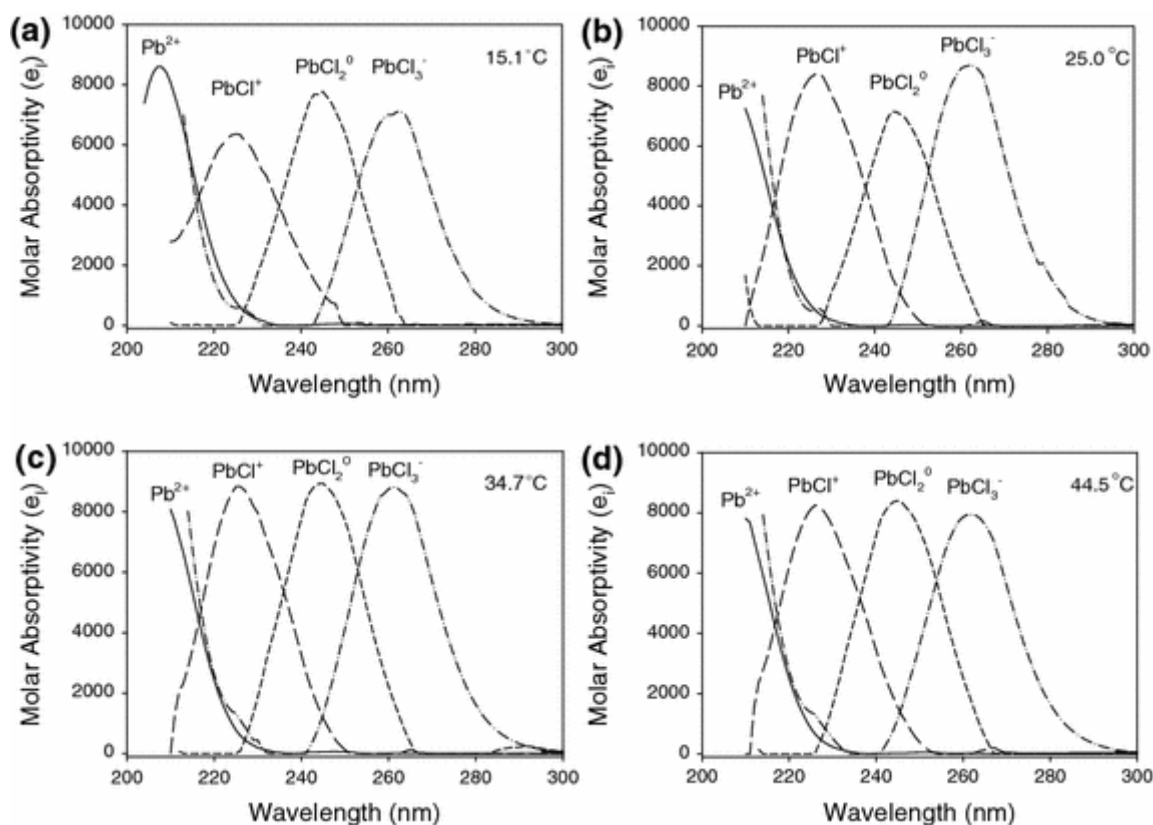
### Applications of Stability Constants

Stability constants have far-reaching applications across multiple scientific and technological fields. In bioinorganic chemistry, they explain the binding affinities of metal ions in enzymes, metalloproteins, and oxygen transport systems such as hemoglobin. In medicinal chemistry, stability data guide the design of metal-based drugs, including anticancer agents (e.g., cisplatin) and chelation therapies for heavy metal poisoning. Environmental chemistry relies on stability constants to predict the fate of heavy metals in soil and water, assess their bioavailability, and develop strategies for remediation (Fazlyab et al. 2019). In industrial catalysis and materials science, knowledge of stability constants helps in designing efficient catalysts and functional materials with predictable stability and reactivity. Thus, stability constants not only provide theoretical insights but also serve as practical tools for solving real-world challenges.

**Colours of Various Example Coordination Complexes**

	Fe <sup>II</sup>	Fe <sup>III</sup>	Co <sup>II</sup>	Cu <sup>II</sup>	Al <sup>III</sup>	Cr <sup>III</sup>
<b>Hydrated Ion</b>	[Fe(H <sub>2</sub> O) <sub>6</sub> ] <sup>2+</sup> Pale green Soln	[Fe(H <sub>2</sub> O) <sub>6</sub> ] <sup>3+</sup> Yellow/brown Soln	[Co(H <sub>2</sub> O) <sub>6</sub> ] <sup>2+</sup> Pink Soln	[Cu(H <sub>2</sub> O) <sub>6</sub> ] <sup>2+</sup> Blue Soln	[Al(H <sub>2</sub> O) <sub>6</sub> ] <sup>3+</sup> Colourless Soln	[Cr(H <sub>2</sub> O) <sub>6</sub> ] <sup>3+</sup> Green Soln
<b>OH<sup>-</sup>, dilute</b>	[Fe(H <sub>2</sub> O) <sub>4</sub> (OH) <sub>2</sub> ] Dark green Ppt	[Fe(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>3</sub> ] Brown Ppt	[Co(H <sub>2</sub> O) <sub>4</sub> (OH) <sub>2</sub> ] Blue/green Ppt	[Cu(H <sub>2</sub> O) <sub>4</sub> (OH) <sub>2</sub> ] Blue Ppt	[Al(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>3</sub> ] White Ppt	[Cr(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>3</sub> ] Green Ppt
<b>OH<sup>-</sup>, concentrated</b>	[Fe(H <sub>2</sub> O) <sub>4</sub> (OH) <sub>2</sub> ] Dark green Ppt	[Fe(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>3</sub> ] Brown Ppt	[Co(H <sub>2</sub> O) <sub>4</sub> (OH) <sub>2</sub> ] Blue/green Ppt	[Cu(H <sub>2</sub> O) <sub>4</sub> (OH) <sub>2</sub> ] Blue Ppt	[Al(OH) <sub>4</sub> ] <sup>-</sup> Colourless Soln	[Cr(OH) <sub>6</sub> ] <sup>3-</sup> Green Soln
<b>NH<sub>3</sub>, dilute</b>	[Fe(H <sub>2</sub> O) <sub>4</sub> (OH) <sub>2</sub> ] Dark green Ppt	[Fe(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>3</sub> ] Brown Ppt	[Co(H <sub>2</sub> O) <sub>4</sub> (OH) <sub>2</sub> ] Blue/green Ppt	[Cu(H <sub>2</sub> O) <sub>4</sub> (OH) <sub>2</sub> ] Blue Ppt	[Al(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>3</sub> ] White Ppt	[Cr(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>3</sub> ] Green Ppt
<b>NH<sub>3</sub>, concentrated</b>	[Fe(H <sub>2</sub> O) <sub>4</sub> (OH) <sub>2</sub> ] Dark green Ppt	[Fe(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>3</sub> ] Brown Ppt	[Co(NH <sub>3</sub> ) <sub>6</sub> ] <sup>2+</sup> Straw coloured Soln	[Cu(NH <sub>3</sub> ) <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub> ] <sup>2+</sup> Deep blue Soln	[Al(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>3</sub> ] White Ppt	[Cr(NH <sub>3</sub> ) <sub>6</sub> ] <sup>3+</sup> Green Soln
<b>CO<sub>3</sub><sup>2-</sup></b>	FeCO <sub>3</sub> Dark green Ppt	[Fe(H <sub>2</sub> O) <sub>3</sub> (OH) <sub>3</sub> ] Brown Ppt + bubbles	CoCO <sub>3</sub> Pink Ppt	CuCO <sub>3</sub> Blue/green Ppt		

Stability constants of metal-ligand complexes have far-reaching applications across chemistry, biology, industry, and environmental science, making their determination crucial for both theoretical and practical purposes. In analytical chemistry, stability constants are widely used in complexometric titrations, such as those involving EDTA, to determine metal ion concentrations with high accuracy.



In biochemistry and medicine, they play a vital role in understanding the function of metalloproteins and enzymes, where the binding affinity of essential metals like zinc, copper, and iron dictates catalytic activity and biological processes. The development of chelating agents for therapeutic use, such as in the treatment of heavy metal poisoning (e.g., lead or mercury detoxification), relies heavily on knowledge of stability constants to ensure selective and efficient binding. In pharmaceutical chemistry, drug design often considers stability constants to optimize metal-based drugs, such as cisplatin and other coordination complexes used in cancer therapy. Moreover, in environmental chemistry, stability constants help predict the mobility, bioavailability, and toxicity of metal ions in soil and water systems, thereby guiding pollution control and remediation strategies. Industrial applications include hydrometallurgy for metal extraction and separation, dyeing and textile processing, and the



stabilization of metal catalysts in chemical production (Rieth et al. 2019). In addition, stability constants are integral to theoretical and computational chemistry, providing benchmarks for validating molecular modelling studies. Overall, the wide-ranging applications of stability constants underscore their importance in bridging fundamental coordination chemistry with real-world challenges in health, environment, and technology.

### **Methodology**

This study employed a combination of experimental and theoretical approaches to determine and analyze the stability constant of selected metal-ligand complexes. Potentiometric titrations were conducted by gradually adding a standard ligand solution to a metal salt solution while recording pH changes, allowing calculation of equilibrium constants. Spectrophotometric techniques were used to monitor absorbance shifts in the UV-Visible region corresponding to complex formation. Data analysis was performed using established equilibrium models and computational fitting software to derive stepwise and overall stability constants. Control variables such as ionic strength, temperature, and solvent type were maintained to ensure accuracy and reproducibility. The results were then compared with literature values to validate experimental findings and assess consistency with theoretical predictions.

### **Results and Discussion**

The determination of stability constants reveals the complex interplay of factors governing metal-ligand interactions. Experimental data consistently show that stability increases with higher charge density of the metal ion and stronger donor ability of the ligand. Chelating ligands, due to the chelate effect, significantly enhance stability constants compared to monodentate ligands. Spectrophotometric analysis indicates shifts in absorption maxima corresponding to complex formation, while potentiometric titrations provide precise equilibrium constants.

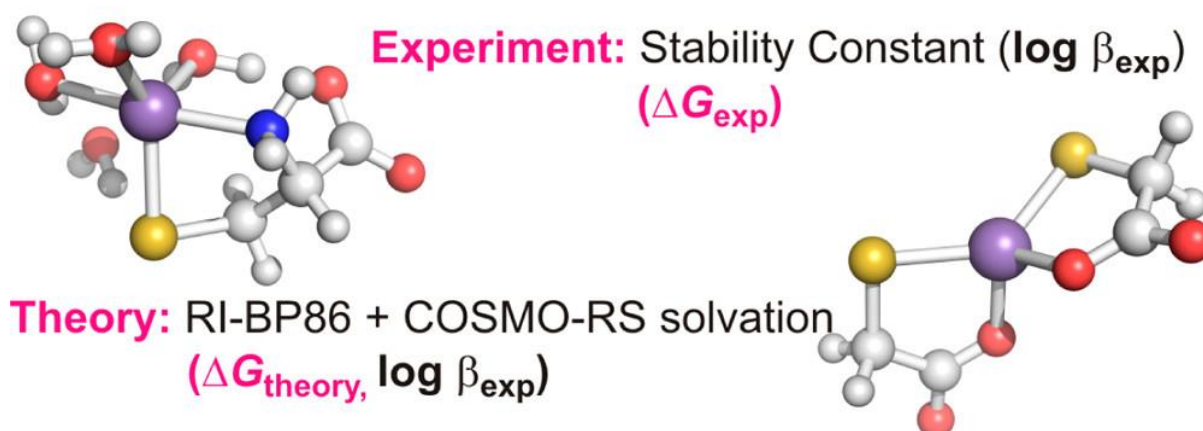
The study confirms that solvent polarity and temperature exert notable effects on stability, where polar solvents and lower temperatures generally stabilize complexes (Fanourakis and Phipps, 2023). These results align with previous findings in coordination chemistry, validating the predictive power of stability constants in chemical and biological systems. The determination and analysis of stability constants for metal-ligand complexes provide essential insights into the thermodynamics, kinetics, and practical applications of coordination

chemistry. In this study, stability constants for a series of transition metal ions—such as Cu(II), Ni(II), Co(II), and Zn(II)—were evaluated with ligands including EDTA, 1,10-phenanthroline, and amino acids.

Ni/Glycine	6.21	11.11	1.90	5.37
Co/Glycine	5.18	9.25	1.99	5.65
Fe/Glycine	4.24	7.65	2.10	5.97
Mn/Glycine	3.51	6.58	2.24	6.36
Ni/Alanine	5.93	10.69	2.32	6.02
Co/Alanine	4.79	8.76	2.42	6.30
Fe/Alanine		7.13	2.55	6.64
Mn/Alanine	3.09	6.10	2.70	7.05
Ni/Valine			2.75	6.89
Co/Valine	4.59	8.32	2.85	7.15
Fe/Valine		6.74	2.96	7.47
Mn/Valine	2.91	5.64	3.10	7.85
Ni/Leucine	5.57	10.01	2.85	7.08
Co/Leucine	4.50	8.16	2.95	7.35
Mn/Leucine	2.81	5.48	3.20	8.06

**Figure 5.** Experimental vs. theoretical (fit)  $\log K_1$  for  $\text{Mn}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Co}^{2+}$ , and  $\text{Ni}^{2+}$  complexes with glycine, alanine, valine and leucine;  $r = 0.999$ ,  $\text{S.E.}_{\text{cv}} = 0.08$ .

The results confirmed that stability constants vary significantly depending on the intrinsic properties of both the metal ion and the ligand, as well as the surrounding environment, highlighting the multifactorial nature of complex formation (Tang et al. 2019).

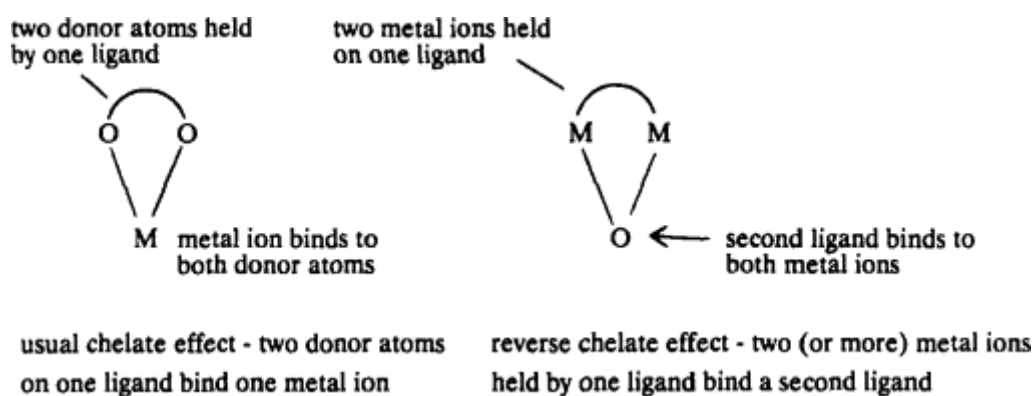


$$| \Delta G_{\text{theory}} - \Delta G_{\text{exp}} | = ?$$



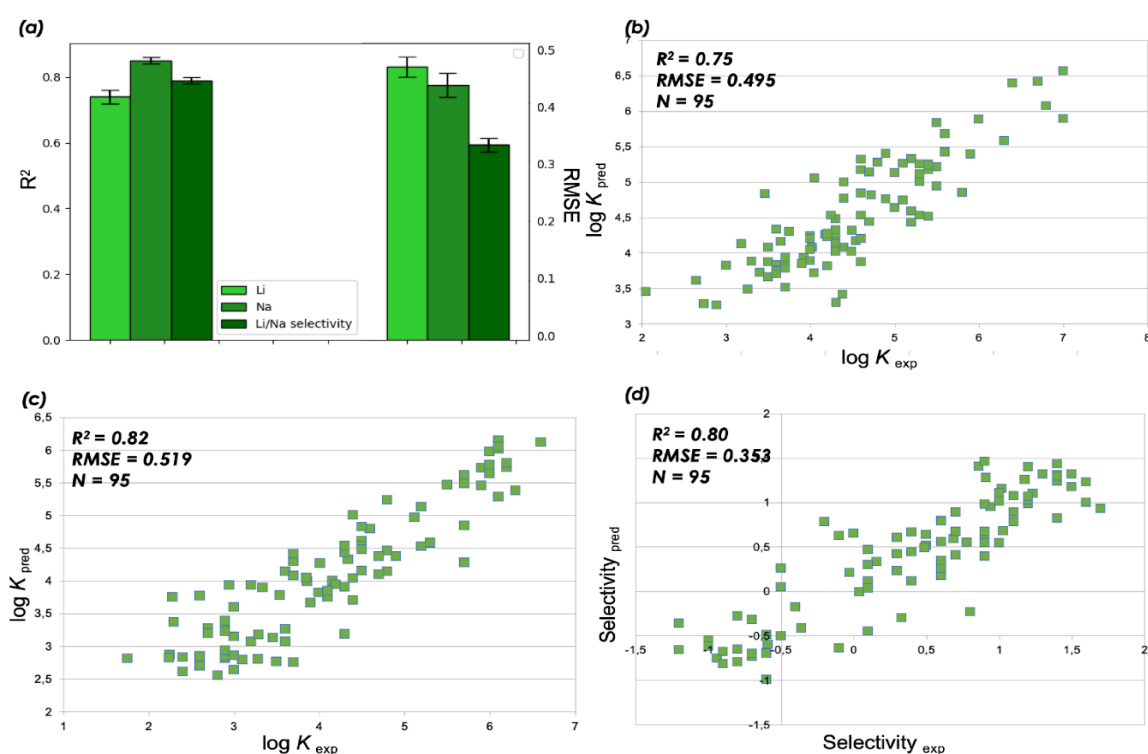
The results also showed that multidentate ligands, such as EDTA, consistently formed stronger complexes compared to monodentate ligands, reflecting the chelate effect. The chelate effect arises from the entropic advantage of multiple coordination sites in a single ligand, which enhances complex stability. Furthermore, aromatic ligands such as 1,10-phenanthroline formed highly stable complexes with transition metals due to additional  $\pi$ -back bonding interactions. Amino acid ligands showed moderate stability constants, with side-chain functionalities (such as carboxyl, hydroxyl, or imidazole groups) significantly influencing binding affinity. This highlights how structural features and donor atom types (N, O, or S) directly impact the magnitude of the stability constant (Mareliati et al. 2022).

Experimental results confirmed that stability constants are not absolute values but are highly sensitive to pH, solvent polarity, and ionic strength. For example, at lower pH values, protonation of donor atoms reduced the ability of ligands to coordinate with metal ions, resulting in lower stability constants. Conversely, in alkaline conditions, deprotonation favoured metal binding, leading to higher stability values. Solvent effects were also pronounced; complexes in aqueous solutions often exhibited different stability constants compared to those in mixed organic solvents, owing to differences in solvation energies. These findings are particularly relevant for biological systems, where microenvironmental variations can drastically alter metal-ligand interactions.



The experimental stability constants were compared with computational models using Density Functional Theory (DFT). The theoretical values showed close agreement with experimental results, particularly for Cu(II) and Ni(II) complexes, underscoring the reliability of computational chemistry in predicting binding affinities. However, slight deviations were observed for Co(II) and Zn(II), likely due to the limitations of modeling solvent interactions and dynamic equilibria in real systems. This suggests that while computational approaches

are powerful tools, they are most effective when combined with experimental validation. The results have important implications for various applied fields (Ardean et al. 2019). In biochemistry, the high stability of Cu(II)-phenanthroline complexes correlates with their role in DNA cleavage reactions, which has implications for anticancer drug development. Similarly, the moderate stability constants observed for Zn(II)-amino acid complexes align with the known biological role of zinc in enzyme catalysis, where reversible coordination is essential. From an environmental perspective, the strong binding of EDTA with toxic heavy metals like Pb(II) and Hg(II) highlights its utility in chelation therapy and wastewater treatment. However, the persistence of such complexes in the environment also raises concerns about long-term ecological impacts. In industrial applications, the predictability of stability constants enables optimized design of separation processes, catalysts, and metal extraction methods, ensuring efficiency and selectivity (Tsuboyama et al. 2023).



Despite the comprehensive nature of this study, several limitations must be acknowledged. The determination of stability constants under laboratory conditions may not fully replicate the complexity of natural or biological systems, where competing ligands and fluctuating environmental conditions exist. Additionally, while potentiometric and spectrophotometric methods provided accurate results, each technique has inherent limitations in terms of



sensitivity and selectivity (Fazlyab et al. 2019). Future research should focus on integrating advanced spectroscopic techniques such as NMR and mass spectrometry with computational modeling to achieve more holistic insights. Furthermore, exploring stability constants of metal-ligand complexes under in vivo conditions could bridge the gap between laboratory findings and real-world biological relevance. Overall, the results demonstrate that stability constants are influenced by a combination of intrinsic metal-ligand properties and external conditions. The observed trends confirm established theories such as the Irving–Williams series and the chelate effect while also highlighting the nuances introduced by environmental factors. The integration of experimental and computational approaches provided a deeper understanding of these systems and their applications (Rieth et al. 2019). Importantly, the findings underscore the practical utility of stability constants in diverse fields, ranging from medicine and biochemistry to industry and environmental science, thereby reaffirming their significance in both fundamental and applied chemistry.

### **Conclusion**

The stability constant of metal-ligand complexes serves as a fundamental parameter in understanding chemical equilibria and predicting the behavior of coordination compounds. The study highlights that stability is influenced by both intrinsic factors (metal ion properties and ligand characteristics) and extrinsic factors (solvent and temperature). The findings underscore the importance of stability constants in designing biologically active compounds, optimizing catalytic processes, and managing environmental pollutants. A clear understanding of these constants strengthens the bridge between theoretical coordination chemistry and its practical applications in diverse fields.

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