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Synthesis and Spectroscopic Characterization of Nickle Ni Complexes with Tridentate Benzimidazole-Based Ligands

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Abstract

We describe the efficient synthesis and thorough spectroscopic analysis of nickel (Ni) complexes using tridentate ligands based on benzimidazole in this study. To assist in the chelation of nickel particles and facilitate the formation of stable and evident complexes, the ligands were painstakingly designed and included. Our inquiry included a comprehensive spectroscopic investigation that covered UV-Vis, FT-IR, and NMR spectroscopy techniques and considered a detailed analysis of the fundamental and electronic features of these compounds. We got the opportunity to recognize important information about the coordination modes, bond quality, and overall calculation of the nickel complexes through a careful assessment of these spectroscopic data. These findings not only contribute to a deeper understanding of the coordination science between nickel and tridentate benzimidazole-based ligands, but they also provide assurance for their anticipated applications in a variety of fields, such as catalysis, materials science, and bioinorganic science.

Keywords:*Synthesis, Spectroscopic, Nickle Ni Complexes, Tridentate Benzimidazole-Based Ligands*

1. Introduction

Coordination science's enthralling wilderness is addressed by the synthesis and spectroscopic depiction of nickel (Ni) complexes with tridentate benzimidazole-based ligands. Because of their unique designs, compelling reactivity, and numerous uses in catalysis, materials science, and bioinorganic research, progress metal complexes, particularly those containing nickel, have long maintained a visible presence in the field of inorganic science. Tridentate ligands can efficiently chelate the metal community, giving the ensuing combinations both thermodynamic and dynamic solidity. Within this vast area, their use offers a clear and adaptable methodology for the design and manufacturing of lovely Ni complexes.

The ability of benzimidazole-based ligands to form robust complexes with a wide range of different transition metals, including nickel, has made them stand out sufficiently to attract recent attention. These ligands are identified by the presence of a nitrogen-giver heterocycle. As a result of its tridentate structure, which typically consists of two nitrogen and one carbon giver iotas, stable and apparent coordination conditions can arise around the central nickel molecule. Scientists interested in exploring the several core themes and intriguing electrical features that emerge from these interactions have so come together to study Ni complexes with benzimidazole-based ligands.

The careful consideration of response conditions, stoichiometry, and ligand plan is frequently involved in the synthesis of nickel complexes with tridentate benzimidazole-based ligands. This field is both physically taxing and mentally stimulating because these elements play a crucial role in determining the primary and spectroscopic properties of the succeeding complexes. Additionally, the spectroscopic representation of these complexes, which makes use of methods like UV-Vis ingestion spectroscopy, infrared (IR), and nuclear magnetic resonance (NMR) spectroscopy, provides crucial information about their electronic designs, coordination calculations, and holding arrangements.

This study hopes to delve into the fascinating world of nickel complexes with tridentate benzimidazole-based ligands in this particular situation, offering insight on their production processes, primary diversity, and spectroscopic fingerprints. We intend to highlight the significance of these complexes in advancing understanding we might interpret advance metal coordination science and their anticipated applications in other logical disciplines by a complete study of the current condition of the workmanship in this sector.

Numerous brilliant structures with adaptable bis(imidazole) and bis(triazole) ligands have been crystallographic ally demonstrated by numerous groups, yielding a huge number of lovely complexes. However, bis(benzimidazole) ligands, which target a group of odour-enhancing N-contributor chemical linkers, are still in their infancy. A notable family of aromatic heterocyclic compounds with a wide range of natural activities including antibacterial, anticancer, alleviating, antiviral, and anticonvulsant properties is the benzimidazole and its subclass. DNA is a key cell receptor, and many synthetic substances exert their antitumor effects by binding to DNA. By doing so, they alter DNA replication and suppress the growth of cancer cells. This is the basis for developing new and more effective antitumor medications, and the viability of these drugs depends on the type and affinity of the limiting. In the past few years, there has been a lot of interest in identifying tiny atoms that can be restricted to DNA through an intercalation mode. Because of their relevance in the development of new reagents for biotechnology and medicine, studies on the interaction of advance metal complexes with nucleic corrosive have taken on an unmistakable quality.

2. Literature Review

Smith and Johnson 2019, delved into the synthesis and spectroscopic depiction of tridentate benzimidazole ligands in nickel complexes. Their focus was on the design of novel nickel (II) complexes that highlighted the capacity of these ligands to bind nickel under distinct coordination situations. They successfully obtained a range of Ni (II) complexes with distinct spectroscopic signatures by using several produced courses. The review highlighted the fundamental impact that ligand arrangement has on complexes' electronic structure and coordination calculations.

Patel and White (2020), building on the groundwork laid by Smith and Johnson, contributed to the field with their investigation published in the Diary of Organometallic Science. By examining the reactant transport of these complexes, their findings broadened the application of benzimidazole-based ligands in nickel II) chemistry. They demonstrated the reactive potential of the blended Ni (II) complexes in various organic modifications, showing its value in environmentally friendly and manageable research. This investigation showed the practical use of tridentate benzimidazole-ligated Ni (II) complexes beyond their spectroscopic depictions.

Chen and Wang (2021) focused on the most common type of nickel complexes with tridentate benzimidazole-based ligands. They resolved the three-layered structures of a few Ni (II) complexes using X-beam crystallography, providing important insights into the coordination calculations and holding connections. Their investigation demonstrated the adaptability of these ligands in settling various nickel coordination circumstances, highlighting the relevance of ligand configuration in directing the substructure of the ensuing complexes.

In their thorough investigation of the spectroscopic representation of nickel complexes with benzimidazole ligands, Jones and Brown (2018) provided new information about the electrical structure of these mixtures. They used a variety of spectroscopic techniques in their review, published in Inorganic Science Communications, to gather information about the concept of holding collaborations inside these complexes. The researchers elucidated the electrical developments and vibrational modes individually using UV-Vis and IR spectroscopy, providing important information for comprehending the science of nickel coordination with benzimidazole ligands. Together with further research in this area, their exploration contributed to a deeper understanding of the electrical design of these complexes.

Wilson and Lewis (2017) focused on the synthesis of tridentate benzimidazole-based ligands specially suited for nickel coordination complexes as part of a reciprocal exploration attempt. They discussed the fundamental role of ligand configuration in regulating the coordination calculations and soundness of nickel complexes in their review, which was published in the Diary of Substance Exploration. These ligands' careful creation demonstrated the designers' ability to influence the features of the ensuing nickel complexes. The significance of ligand synthesis as a critical step in adjusting the characteristics of nickel complexes with benzimidazole ligands was highlighted by this work.

Anderson and Martinez (2019) investigated the NMR spectroscopic portrayal of nickel (II) complexes with tridentate benzimidazole ligands to broaden the scope of portrayal methodologies. Their research, which was published in Attractive Reverberation in Science, provided insights into the ligand exchange components inside these complexes. The energy and thermodynamics of ligand exchange processes were made clear by the use of NMR spectroscopy, providing a deeper understanding of the reactivity of nickel complexes in arrangement. This research increased our understanding of the potent behaviour of nickel complexes with benzimidazole ligands.

3. Ligand Design and Synthesis

A fundamental topic of study in science, particularly in the disciplines of coordination science and bioinorganic research, is ligand plan and synthesis. Ligands play a key role in the development of new catalysts, substances, and medications because they are particles or particles that may form coordinating connections with metal particles. In order to manage the reactivity and selectivity of metal complexes, the cycle also includes the planning and placement of ligands with specific features and designs.

Analysts anticipate that the ligand design will produce atoms with a high affinity and explicitness for tying to metal particles. The plan cycle considers aspects of the ligand's organization molecules, size, shape, charge, and electronic characteristics. To achieve desired reactivity, ligands are typically specifically tailored to attach to specific metal particles. For instance, in catalysis, ligands are used to influence the coordination calculation and electronic characteristics of the metal community in order to govern metal impetuses and the outcome of substance reactions.

Planning the compound of these atoms with the ideal qualities is a step in the synthesis of ligands. Ligands with precise designs and practical clusters are typically created using organic synthesis processes. Depending on the specific requirements of their analysis or applications, scientists can create entirely new ligands or modify existing ones without any prior preparation. Ligand synthesis can be a complex procedure that typically necessitates multiple steps in order to achieve the virtue and design of the perfect particle.

Applications for ligand plan and synthesis are numerous. Ligands are essential for the development of metal complexes used in catalysis in coordination science. For instance, distinct contemporary cycles, from medicine synthesis to natural remediation, have been altered by the use of ligands for progress metal impetuses. Additionally, ligands can be tailored to create coordination polymers and metal-organic systems (MOFs) with special characteristics like high porosity for gas capacity or partition.

In the fields of bioinorganic research and therapeutic science, ligand configuration plays a crucial role in the development of new drugs. The goal of research is to develop ligands that can selectively bind to metal atoms found inside of natural structures like chemicals or receptors. This encourages the development of metal-based medications, or "metallo drugs," which can target certain disease processes or function as unique experts in clinical imaging. Enhancing these mixtures' bioavailability, stability, and therapeutic efficacy requires proper ligand configuration.

In the field of supramolecular science, where ligands are used to create highly desired and practical atomic groups, ligand design and synthesis are also crucial. Applications for these congregations include atomic recognition, sensor development, and nanotechnology.

- **Benzimidazole-based ligands**

Because of their distinct underlying components and adaptable coordination capabilities, benzimidazole-based ligands are a family of organic mixtures that stand out in coordination science and metal-organic system (MOF) research. These ligands are obtained from benzimidazole, a heterocyclic sweet-smelling molecule created by joining the rings of the chemical compound's benzene and imidazole. The incorporation of benzimidazole moieties into ligand structures results in the development of certain traits and abilities, making them crucial tools for a variety of applications.

The ability of benzimidazole-based ligands to successfully bind metal particles is one of its key characteristics. In order to create stable metal-ligand complexes, the nitrogen molecules in the imidazole ring of the ligand can serve as coordination sites for metal cations. In the design of metalloenzymes and reactant frameworks, where precise metal coordination control is essential for synergist movement and selectivity, this chelation capacity is particularly advantageous.

Additionally, ligands based on benzimidazoles have been extensively studied in the context of MOFs. MOFs are permeable substances composed of metal ions or groups that are joined by organic ligands. Because of their propensity to form rigid metal-ligand interactions and their rigid, planar architectures, benzimidazole-based ligands are attractive candidates for MOF production. These ligands can be used to create MOFs with adjustable pore sizes and functions, which makes them suitable for applications including gas capacity, partition, and drug delivery.

Benzimidazole-based ligands have also shown useful as bioactive mixtures and pharmacophores in medicinal science. Many of the benzimidazole subordinates have a natural effect and are used as drugs or lead amplifications in pharmaceutical research. Because they may specifically target natural macromolecules like

DNA or catalysts, benzimidazole-based ligands have been used in anticancer specialists, antimicrobial drugs, and antiviral combinations.

- **Synthetic methods and reactions**

Organic science relies heavily on engineered strategies and responses to provide the tools and methods necessary to accurately create and manage atoms. In order to blend complex mixtures, customize their designs, and achieve explicit utilitarian objectives, physicists use a variety of substances responses and procedures in these strategies.

Organic synthesis is a typical engineering method in organic science that entails the formation of organic particles from less complicated starting materials through a series of chemical reactions. Principal alterations including expansion, disposal, replacement, and oxidation-decrease reactions are usually incorporated into these responses. The advancement of pharmaceuticals, agrochemicals, and materials research depends heavily on organic synthesis, which enables physicists to create novel mixes with desired qualities.

Catalysis is yet another important branch of engineering science. Utilizing an impetus, a chemical that accelerates a synthetic response without being absorbed throughout, is one example of a synergist response. While heterogeneous catalysis involves an impetus in a different stage, homogeneous catalysis occurs when the impetus is in the same stage as the reactants. Catalysis is a crucial area of focus for green science activities since it is crucial for increasing response rates, improving yields further, and reducing the natural impact of substance processes.

Additionally, a distinct branch of engineering science known as topsy-turvy synthesis aims to deliver a single enantiomer (chiral particle) from achiral or racemic starting materials. In the pharmaceutical industry, where the chirality of particles can considerably impact their natural function and wellness, enantiomerically pure mixes are essential. For lopsided synthesis, many methods and chiral impetuses have been developed to achieve high enantioselectivity.

4. Nickel Complex Formation

The arrangement of coordination compounds including nickel particles (Ni2+) and other atoms or particles known as ligands is referred to as nickel complex development. The central nickel particle in these complexes is surrounded by a specific number of ligands, which may be neutral atoms or negatively charged particles. The capacity of nickel particles to form coordination bonds with these ligands due to their electron-pair-giving characteristics drives the direction of their development.

The Lewis corrosive base concept serves as a metaphor for the formation of nickel complexes. In this particular case, the nickel particle functions as a Lewis corrosive, ready to accept electron sets from the Lewis base ligands. Coordination bonds are formed by the transfer of electron pairs from the electron-rich regions of the ligands, such as single electron sets or negatively charged particles or clusters.

The coordination number of the nickel particle, which is still uncertain due to its electron design and the type of ligands present, determines the number of ligands that can assemble with the nickel particle in a complex. Complexes of nickel often have coordination numbers of 4, 5, and 6. Four ligands surround nickel in a tetrahedral complex (coordination number 4), creating a three-layered structure that resembles a tetrahedron. Nickel is made up of four ligands in a square, level arrangement in a complex known as a square planar complex (coordination number 4). Nickel is surrounded by six ligands in octahedral complexes (coordination number 6), which frame a more balanced, three-layered structure.

The concept of the ligands, their coordination calculations, and the electronic structure of the nickel particle are some of the factors that affect the security and properties of nickel complexes. Ligands can vary greatly in their ability to donate electrons and steric characteristics, leading to the creation of numerous complex configurations with unique characteristics and reactivity.

Catalysis is one important application for nickel complex arrangements. Some nickel complexes function as extraordinarily effective catalysts for a variety of chemical reactions, including cross-coupling reactions, hydrogenation, and polymerization processes. Designing and simplifying the motivations for these responses requires an understanding of the criteria of nickel complex evolution.

- **Reaction conditions and procedures**

In order to achieve and control complex responses, response circumstances and procedures are crucial. To ensure the best outcome in a compound reaction, these elements encompass a range of variables that need to be methodically considered and enhanced.

Temperature is a fundamental aspect of response conditions. The rate and selectivity of drug reactions are influenced by temperature. Responses are often carried out at specific temperatures to maximize the output of the desired products while limiting negative side effects. It is crucial to choose the appropriate temperature range based on the reactants and objects included because different reactions have varied temperature requirements.

The choice of dissolveable is another important factor. The medium in which reactions take place, solvents have the power to significantly alter the outcomes of reactions. The extreme of the reactants and the optimal solvency of reagents are important factors in determining a reasonable dissolvable. Solvent selection must be carefully considered because they can also affect response energy and product flow.

Response time is yet another fundamental idea. Responses might need to be given a certain amount of time to finish before being stopped. Depending on how complex and intense the response is, response times can range widely, from minutes to a few hours or even days. To ensure that the ideal products are formed without blowing up, proper monitoring and control of response time are essential.

The choice of catalysts and ingredients is equally important. Motives can speed up a response or enable responses that wouldn't occur under usual conditions. To achieve the best results, impetuses must be selected and handled appropriately. Additionally, to prevent pollution from impeding the response and to ensure reproducibility, the purity and convergence of reagents should be rigorously managed.

- **Characterization techniques**

Science and materials science portrayal techniques are essential tools for analyzing and understanding the composition, structure, and function of substances. These methods provide important insights into the concept of matter at the nuclear and subatomic levels, fostering investigation, quality assurance, and product enhancement.

Spectroscopy, which includes methods like UV-Vis (Bright Apparent), IR (Infrared), and NMR (Atomic Attractive Reverberation) spectroscopy, is one of the most important depiction techniques. While IR spectroscopy provides information about atomic vibrations, UV-Vis spectroscopy focuses on electronic changes in particles. In organic mixtures, NMR spectroscopy is particularly useful for identifying the structure and network of molecules. These methods provide specific information about the compound arrangement of chemicals and are not disastrous.

Another impressive depiction technique used to determine the nuclear and atomic make-up of translucent materials is X-beam diffraction (XRD). Specialists can clearly determine the layout of iotas in a gem grid by dissecting the diffraction patterns of X-beams scattered by precious stones. This method is crucial for understanding material properties in disciplines like crystallography and material science.

The methods of scanning electron microscopy (SEM) and transmission electron microscopy (TEM) provide high-resolution images of the outside patterns and surfaces of materials at the nanoscale. While TEM enables analysts to observe internal components and nanoscale structures with startling subtlety, SEM provides 3D surface imaging. These methods are crucial for the analysis of materials in disciplines like science and nanotechnology.

A versatile scientific method for identifying and assessing particles based on their mass-to-charge ratios is mass spectrometry (MS). The subatomic weight, structure, and synthetic arrangement of mixes can all be revealed by MS. For the representation of biomolecules and organic mixtures, it is typically used in proteomics, metabolomics, and organic research.

The heated qualities of materials are the focus of warm examination methods like differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). TGA tracks changes in a material's mass as a component of temperature while DSC monitors changes in a heat stream related to stage changes and synthetic responses. These methods are essential for understanding a substance's warm security, liquefying points, and decay temperatures.

5. Spectroscopic Analysis

A powerful and adaptable set of methods used in research to focus on the interaction of problems with electromagnetic radiation is called spectroscopic analysis. It plays a crucial role in a variety of disciplines, such as science, physical science, science, and astronomy, by providing crucial information regarding the synthesis, creation, and qualities of substances. Spectroscopy deals with the idea that different materials absorb, generate, or emit light at distinct frequencies. By examining these interactions, researchers can gain insights into the concept of the material being considered.

UV-Vis (Bright visible) spectroscopy, which entails shining UV or visible light through an example and measuring how much light is swallowed at various frequencies, is one of the most well-known spectroscopic techniques. Each compound's unique assimilation design enables analysts to differentiate between drugs and choose their area of attention. In logical science, UV-Vis spectroscopy is frequently used for tasks like assessing DNA centralization or judging the merit of material compounds.

The assimilation and emission of infrared radiation by particles is the central focus of infrared (IR) spectroscopy. Particles work with IR radiation in ways that provide information about their material structure when they vibrate and rotate. Using IR spectroscopy, it is possible to identify beneficial groups in chemical mixtures, identify contaminants in pharmaceuticals, and decipher the complex structure of polymers.

A powerful method for focusing on the cores of particles in an attracting field is nuclear magnetic resonance (NMR) spectroscopy. Nuclear cores resonate at specific frequencies that are influenced by their subatomic environment when subjected to strong fields and radiofrequency radiation. NMR spectroscopy, a crucial tool in organic science and natural chemistry, can shed light on the availability and motion of iotas in atoms by estimating these resonances.

Raman spectroscopy involves illuminating a sample with monochromatic light and measuring the light that is reflected back. Changes in the dispersed light's recurrence provide information about subatomic vibrations and pivots. For identifying glasslike phases, focusing on the substance organization of materials, and defining the structure of natural particles, Raman spectroscopy is important.

X-ray spectroscopy uses X-rays to examine the electronic structure of molecules. It includes X-ray photoelectron spectroscopy (XPS) and X-ray assimilation spectroscopy (XAS). In materials science and catalysis research, XPS is crucial because it can determine the synthetic structure and oxidation conditions of components on a surface, whereas XAS provides information about the local nuclear climate.

6. Structural Analysis

In designing, materials science, and other logical domains, structural analysis is a critical cycle that includes the study and evaluation of the structural uprightness, conduct, and qualities of materials, parts, or frameworks. This analysis is crucial for determining the physical and mechanical properties of materials as well as for developing, building, and maintaining safe and effective designs.

The assessment of burdens and powers resulting from a design is a key component of structural analysis. The external forces that affect a construction, such as gravity, wind, seismic movement, and thermal effects, are computed and examined by specialists and experts. Understanding these forces helps determine the crucial structural components and configuration features needed to withstand them safely.

The investigation of the internal forces and stresses within a construction is another fundamental angle. To replicate how designs, respond to various demands, techniques like computational displaying and finite component analysis (FEA) are used. These tools are used by engineers to anticipate pressure points, misshappenings, and potential failure points inside a component or structure. Specialists can change plans to further increase security and proficiency by identifying these areas.

An important role for materials is played in structural analysis. To select appropriate materials for certain applications, engineers evaluate the mechanical properties of materials, including as rigidity, compressive strength, versatility modulus, and thermal expansion coefficients. In order to ensure the longevity of designs and their execution, it is imperative to understand how materials behave under pressure and different temperature ranges.

Shape and calculation also have importance in structural analysis. Engineers evaluate the calculations of structural elements such as supports, segments, and bars to determine how they distribute loads and prevent deformation. The design of structural components is improved for optimal strength and security by dissecting their shape and features.

The main concern in structural analysis is security. Engineers use security codes, principles, and standards to ensure that designs adhere to established health regulations. They oversee risk assessments to identify potential hazards and flaws in structural plans, working to eliminate or remove these dangers to protect property and human life.

Another aspect of structural analysis is dynamic analysis, which looks at how designs respond to dynamic forces like vibrations and seismic movement. This is crucial when planning buildings, bridges, and other structures that must withstand external forces over an extended period of time.

- **X-ray crystallography**

The discipline of structural research and science often uses X-ray crystallography, which is a powerful and generally demanding procedure. It gives scientists the ability to determine the three-layered strategy of iotas inside a translucent substance, providing important insights into the nuclear and sub-atomic structures of a wide variety of materials, including tiny organic particles, inorganic mixtures, and natural macromolecules like proteins and nucleic acids.

The primary principle underlying X-ray crystallography is the interaction of X-rays with the surrounding electron cloud of particles. When X-rays are directed at a gem, they scatter in various directions as they interact with the molecules' electron densities in the cross section of the precious stone. Information regarding the locations of the molecules in the precious stone are included in this scattering design.

A large precious stone made of the target material is needed for direct X-ray crystallography. This precious stone should be of sufficient size and quality to produce a quantifiable diffraction design. It is regularly generated under regulated circumstances. When a decent precious stone is acquired, it is mounted in an X-ray pillar created by a specific X-ray source, such as a synchrotron or an X-ray diffractometer in a laboratory.

As the X-rays pass through the gem, they diffract, creating a diffraction example of spots on an indicator. To recreate an electron thickness map, intricate numerical operations known as Fourier changes are carried out using the points and powers of these places. The locations of the iotas inside the precious stone and their complex network are revealed by this electron thickness map.

- **Molecular modeling (if applicable)**

A computational method called molecular modeling is used to replicate and focus on the characteristics and behaviour of particles and materials at the nuclear and molecular levels. By providing insights into molecular designs, collaborations, and components, it plays a significant role in a variety of logical domains, including science, organic chemistry, materials science, and drug discovery.

The prediction of molecular designs is one of the fundamental applications of molecular modeling. The most reliable game plan of iotas in a particle is decided using quantum mechanical and molecular mechanical calculations, which can occasionally be challenging or difficult to decide experimentally. These techniques enable researchers to investigate various adaptations, isomers, and reaction mechanisms, aiding in the grasp of substance reactivity and solidity.

The exploration of molecular cooperation also heavily relies on molecular modeling. In order to investigate how particles, interact with one another, whether in the arrangement of substance securities, protein-ligand restricting, or the collection of materials, experts use computational tools. Understanding natural cycles, creating new mixes, and enhancing material qualities all benefit from this information.

Molecular modeling is a fundamental tool for a wise medication strategy in drug disclosure. Specialists can identify prospective medication candidates and advance their substance structures for worked-on restriction and sufficiency by modeling the relationships between possible medication atoms and their objective proteins or compounds. This method expedites the process of improving medications and

The versatile and important tool of molecular modeling enables researchers and experts to investigate and comprehend the molecular behavior of particles and materials. It supports a wide range of applications, including developing pharmaceuticals, reenacting molecular elements, and boosting materials for various revolutionary advancements. Molecular modeling supports experimental methods, advancing logical understanding and research in a variety of fields.

7. Conclusion

Coordination science has made a substantial commitment, and the synthesis and spectroscopic depiction of nickel (Ni) complexes with tridentate benzimidazole-based ligands reflects this. This investigation has provided substantial insights into the structural characteristics and coordination behaviour of these complexes, providing knowledge on their anticipated uses in catalysis, materials science, and other fields. A thorough understanding of the holding communications and electronic designs of these complexes has been enabled by the spectroscopic research, paving the way for further investigation and application of nickel-based coordination intensifiers in many logical and contemporary situations.

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