

Synthesis and Characterization of Coordination Compounds with Novel Ligands: Implications for Material Science

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Abstract - Coordination compound are any of a class of substances with produced plans where a central metallic particle is encircled by non-metal elements or social assemblies of particles, termed ligands. A basic use of coordination compounds is their use as motivations, which effectively change the speed of designed responses. This study researches the mix and depiction of coordination compounds incorporating novel ligands, with an accentuation on their ideas for material science. Coordination compounds, outlined by the coordination of a central metal atom or molecule with various ligands, are crucial for an extent of engineered and present day cycles. In this investigation, we detail the mix of a couple of coordination compounds featuring as of late made ligands. These ligands are planned to give express electronic and steric influences, smoothing out the introduction of the ensuing edifices.

Keywords: Synthesis and Characterization, Coordination Compounds, Novel Ligands

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INTRODUCTION

Coordination chemistry was established by Swiss researcher A. Werner (1866-1919), who won Nobel Prize in 1913. Extraordinary commitment was additionally made by Russian scientific expert L.A. Chugaev (1873-1922). Coordination (complex) elements comprise of a cationic, anionic, or impartial complex, containing a focal particle or particle and atoms or particles, facilitated with it. Those substances, whose particles contains a focal molecule, associated with ligands, can be considered as coordination or complex elements. In this multitude of compounds, the cations are encircled with anions, nonpartisan particles or extremists. The gatherings, encompassing straightforwardly the cation, are named ligands; the area of inorganic chemistry, concentrating on joint way of behaving of cations and their ligands, was named as coordination chemistry.

In most coordination compounds it is feasible to distinguish a focal or center iota or particle that is reinforced not just to another molecule, particle or gathering through a direction bond, yet to a few of

these elements immediately. The focal molecule is an acceptor, with the encompassing species each getting (in any case) one single plans of electrons to accommodate a void orbital on the focal particle, and this electron couple supports known as a ligand related.

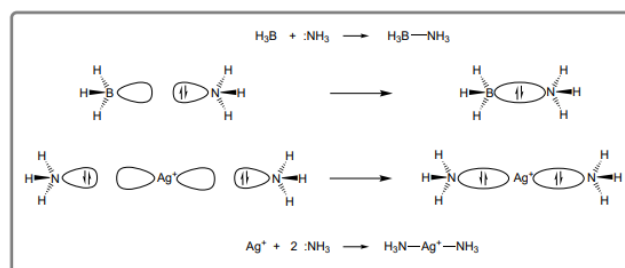


Figure 1 A schematic perspective on smelling salts going presumably supplier ligand to a metalloid acceptor and to a metal particle acceptor to move toward coordinate bonds.

The class giving the electron couple considered existence made for classes getting solitary plans of electrons. These organizing substance ligand, can

be fundamentally basically little monatomic atom or wide polymer - the crucial brand name stands the occurrence of something like solitary plans of electrons on an electronegative ally molecule. Supplier iotas from time to time encountered remain hetero particles similar N, O, S and P in addition to halide particles, so far it is in no way, shape or form at all, the full reach. Additionally, overwhelmingly most of existing standard particles can go about as ligands, or, almost certainly can be changed over into particles fit for going about as ligands. A traditional and strong ligand is smelling salts, NH₃.

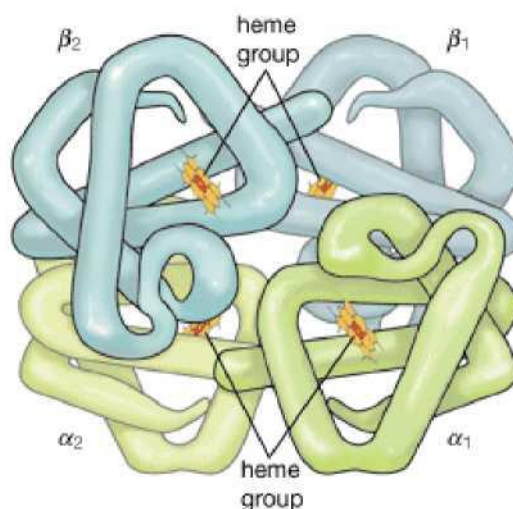
Coordination compounds are basic for no obvious reasons. Regardless, the majority of the parts in an occasional table are metals, and essentially all metals structure structures, so metal designs are a part of the chemistry of the bigger part the parts. Second, different current impetuses are metal designs, and such boosts are dependably turning out to be more basic as a strategy for controlling reactivity. For instance, a blend of a titanium magnificent and an organometallic compound of aluminum is the impetus used to convey by a long shot the vast majority of the polyethylene and polypropylene "plastic" things we use dependably. At last, progress metal designs are pivotal in biochemistry. Models solidify hemoglobin, an iron complex that transports oxygen in our blood; cytochromes, iron designs that move electrons in our cells; and designs of Fe, Zn, Cu, and Mo that are essential bits of unequivocal manufactured compounds, the boosts for every regular response.

COORDINATION COMPOUNDS IN CHEMISTRY

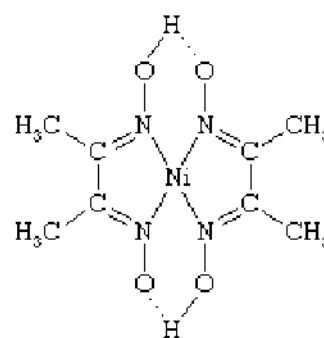
Expectedly happening coordination compounds are basic for living customary substances. Metal designs play different colossal circumstances in conventional plans. Coordination compounds are a fascinating and crucial area in chemistry, particularly within the field of inorganic chemistry. They consist of a central metal atom or ion bonded to surrounding molecules or ions, known as ligands. These compounds have a wide range of applications, from catalysis and material science to medicine. Understanding coordination compounds requires knowledge of both their chemical bonding and their physical and chemical properties, which can be quite complex due to the variety of possible ligands and metal centers.

Coordination compounds can indeed display a remarkable range of colors, which make them valuable not only in scientific contexts but also in applications like dyes and pigments. The vivid colors observed in many coordination compounds are primarily due to electronic transitions within the metal ion's d-orbitals.

When ligands interact with the metal ion, they split the d-orbital energies into different levels. This splitting causes the metal complex to absorb certain wavelengths of light, and the complementary color of the absorbed light is what we perceive. Phthalocyanines, such as copper phthalocyanine, are another class of coordination compounds known for their vibrant and stable colors. These compounds consist of a large, conjugated macrocyclic ring system that binds to a metal ion, often copper. The structure is similar to that of porphyrins, which are also large, ring-shaped ligands. (1) Copper Phthalocyanine (CuPc): This compound is widely used as a pigment in paints and textiles. Its deep blue-green color results from extensive delocalization of π -electrons across the ring system and metal center. (2) Porphyrins: These are another class of macrocyclic compounds with a ring structure that binds to metal ions. Hemoglobin and chlorophyll are natural examples. Synthetic porphyrins are used in dyes, catalysts, and medical imaging.



There are several behaviors by means of coordination compounds remain utilized upon investigation of changed materials. The incorporate (1) particular rainfall of metal atoms as structures — for example, nickel(2+) atom as the dimethylglyoxime compound



(2) the course of action of concealed structures, for instance, the tetrachlorocobaltate(2-) molecule,

which can be settled spectrophotometrically — that is, through their light ingestion properties, and (3) the preparation of buildings, for instance, metal acetylacetonates, which can be detached from watery plan by extraction with regular solvents.

In unambiguous circumstances, the presence of metal particles is sad, as, for example, in water, in which calcium (Ca^{2+}) and magnesium (Mg^{2+}) ions cause hardness. In such cases the miserable impacts of the metal atoms some killed by "sequester" these atoms as innocuous structures improvement for fitting complexion substance. Ethylenediaminetetraacetic horrendous shapes most likely constant designs. Its applications unite water advancing (by tying up Ca^{2+} and Mg^{2+}) also, the protection of standard materials.

A machine-driven and steady development basic openness in 1954 that precise compound iron motivations — explicitly, a mixture of TiCl_3 , and $\text{Al}(\text{C}_2\text{H}_5)_3$ — accomplish the polymerizations of standard compounds through carbon double bonds underneath fragile situations to figure polymers of high nuclear mass and essentially referenced (stereoregular) architecture. You've touched on some significant areas in polymer chemistry and catalysis. Many polymers are crucial in manufacturing various products. For instance, polymers like polyethylene and polypropylene are used in everything from packaging films to automotive parts. **The Hydroformylation** process involves the reaction of olefins with hydrogen and carbon monoxide to produce aldehydes. Metal carbonyls, such as hydridotetracarbonylcobalt, play a vital role in this reaction. It's an important industrial process for producing aldehydes that are used in a variety of chemical syntheses. **The Oxidation of Ethylene**, Tetrachloropalladate(2-) ions are catalysts used in the oxidation of ethylene to produce acetaldehyde. This reaction is significant in the production of chemicals used in various applications, including the synthesis of acetic acid and other derivatives. These processes are integral to producing chemicals and materials that are foundational to many industries, highlighting the importance of understanding and optimizing these catalytic systems for efficient and sustainable production.

WERNERS' COORDINATION THEORY

Coordination complexes were identified in 1800 years. This one classified legitimate expert, to get a handle on concerning why a steady salt like CoCl_3 replies with fluctuating number of stable particles or compounds, for example, solvent base to give two or three new compounds $\text{CoCl}_3 \cdot 6\text{NH}_3$, $\text{CoCl}_3 \cdot 5\text{NH}_3$ and $\text{CoCl}_3 \cdot 4\text{NH}_3$; This complexes separated since one another atom reactivity. conductivity appraisals on courses of action of this complexes indicated that

how much particles current in answer for every complex are remarkable. Numerous hypotheses were suggested, yet no one can sufficiently sort out enormous number of obvious possessions of this complexes and comparative additional sequences of complexes which had been coordinated. It was absolutely in 1893 that Werner set forth ton of contemplations which are identified as per Werner's co-ordination hypothesis, sort out holding in structures.

The immense appraisals of Werner's hypothesis are:

1. Metals show two sorts of valence:
 - (a) Key valence (ionizable)
 - (b) Aide valence (non-ionizable).

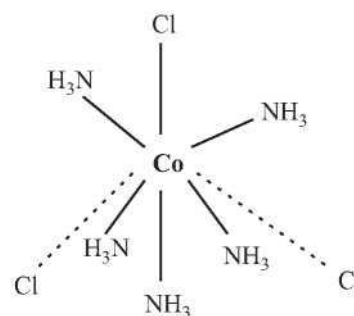
Key is fulfilled through lamentable particles then associates with corrosion condition of the iron. The optional valence, which is fulfilled by woeful, honest social events, indistinguishable from the co-ordination amount of metallic atom.

Each metal will generally fulfill the two its essential and colleague valence.

2. The associate valence is worked with near immovable locations in universe for example this has spatial game plan associating with various coordination number.

Structures $\text{CoCl}_3 \cdot 6\text{NH}_3$, $\text{CoCl}_3 \cdot 5\text{NH}_3$ and $\text{CoCl}_3 \cdot 4\text{NH}_3$ the amount of ionizable particles in this structures are 3, 2 and 1, independently. It has been exhibited by rainfall responses and conductivity assessments. In view of Werner's speculate these compounds are arranged as:
 $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$, $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$ and $[\text{Co}(\text{NH}_3)_4\text{Cl}_2]\text{Cl}$, independently.

In light of Werner's speculation the development of $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$ is:



Primary valence (ionizable)(.....)

Secondary valence (non-ionizable) (-----) Holding is a critical piece of the time depicted utilizing the formalisms of atomic orbital theory.

Individual of the three chloride particles fulfill both essential and auxiliary valence.

Six facilitated edifices, for example, $[\text{Ni}(\text{NH}_3)_6]^{2+}$ and $[\text{Co}(\text{NH}_3)_6]^{3+}$ are

THE ROLE OF LIGANDS IN COORDINATION CHEMISTRY

Coordination chemistry, the science worried about the joint exertion of typical/inorganic ligands with metal focuses has stayed one of the most impressive evaluation regions in inorganic chemistry. Coordination chemistry combines various types of coordination compounds important in a wide variety of fields like tones, colors, atomic powers, catalysis, photography, toxicology, bioinorganic chemistry, drug, pottery creation, materials science and toxicology. Considered different ligands in structures has empowered their applications as biocides, upgrades, NMR shift reagents and DNA covers. The improvement of current intelligent instruments and relationship of a wide assortment of coordination compounds has urged different specialists to return to the substance responses. This study has empowered the inorganic consistent experts to gain fundamental headway in the change of the chance of designed holding.

In coordination chemistry, the various types of ligands, Schiff base ligands and chelates are genuine with blend, portrayal and applications. The designs of progress metals with higher nuclearity stand sufficiently separated to be seen of different coordination coherent trained professionals, where polytopic ligands are colossal for tailor made sub-atomic arrangements of designs. The polytopic ligands are unimaginably improved for the practical course of action of the homo polynuclear structures notwithstanding, the one-pot mix for the readiness of polynuclear structures is especially disappointed. To work with the tailor making of heterometallic structures in a controlled way and with expected properties, the best concern is the improvement of planned courses. From among the extent of systems, the utilization of metal structures as ligands has displayed to gain genuine headway. On the off chance that the designs shaped by coordination with metal particles, will by and large work with further or reply with different structures, then, they could go about as 'metal typical ligands'.

As a rule, are seen as electron suppliers and the metals as electron acceptors, i.e., freely, Lewis bases and Lewis acids. This depiction has been semi-assessed in different ways, for example ECW model.

Ligands and metal particles can be referenced in different ways; one arranging framework rotates around ligand 'hardness' (see moreover hard/delicate horrendous/base theory). Metal particles especially tie and $[\text{Ni}]$ unequivocal ligands. If all else fails, 'hard' metal particles favor delicate field ligands, notwithstanding 'touchy' metal particles incline strong regions for toward ligands. As indicated by the atomic orbital theory, the HOMO (By and large significant Involved Sub-atomic Orbital) of the ligand ought to have an energy that covers with the LUMO (Least Void Atomic Orbital) of the metal explicit. Metal particles headed strong regions for to ligands keep the Aufbau rule, but structures bound to weak field ligands go along to Hund's standard.

Restricting of the metal with the ligands accomplishes a ton of sub-atomic orbitals, where the metal can be associated with another HOMO and LUMO (the orbitals depicting the properties and reactivity of the following staggering) and a specific referencing of the 5 d-orbitals (which might be filled, or somewhat piled up with electrons).

Holding Speculations

To make sense of the plans, solid qualities and general properties of the co-ordinated compounds following hypotheses are utilized.

1. Crystal Field Theory (CFT)

2. Ligand Field Theory (LFT)

1. Crystal Field Theory (CFT)-

Despite what the way that valence bond speculation sorts out the holding and associating with properties of plans, it is bound in two immense ways. Anyway, the speculation can with crucial effort sort out the shade of plans. Second, the speculation is endeavoring to quantitatively develop. In that limit, another speculation — crystal field theory — has arisen as the overall perspective on change metal plans.

Crystal Field Theory was advanced by Hans Bethe and John Hasbrouck van Vleck. Their work in the mid-20th century provided a quantitative approach to understanding the electronic structure of transition metal complexes. CFT explores how the presence of ligands affects the energy levels of the d-orbitals in a metal ion. In this theory, ligands are treated as point charges or dipoles that create an electric field

around the central metal ion. In the simplest models, ligands are considered as point charges, with anionic ligands contributing negative charge and neutral ligands providing a dipole effect. This approach simplifies the calculation of the ligand field's impact on the metal ion's d-orbitals. Crystal Field Theory offers a model to understand how the spatial arrangement and electronic environment created by ligands influence the energy levels of a metal ion's d-orbitals. This theory has had a profound impact on our understanding of coordination chemistry and the behavior of transition metal complexes.

The impact of an octahedral field on the d-orbitals of a metal ion is a central concept in Crystal Field Theory (CFT). In a free metal ion, the five d-orbitals are degenerate, meaning they all have the same energy. In an octahedral complex, six ligands are arranged around a central metal ion in an octahedral geometry. The ligands are positioned along the axes of the metal ion, creating an octahedral electric field. Fig. 2 indicates the states of the 5 d orbitals. Survey that this shape really focuses on the volume no inquiry going for involved by electron containing orbital. The another 4 d orbitals take "cloverleaf" figures, every changing from each other fundamentally toward the turns in space. The "cloverleaf" orbital $dx^2 - y^2$ has its turns along the x-axis and the y-focus.

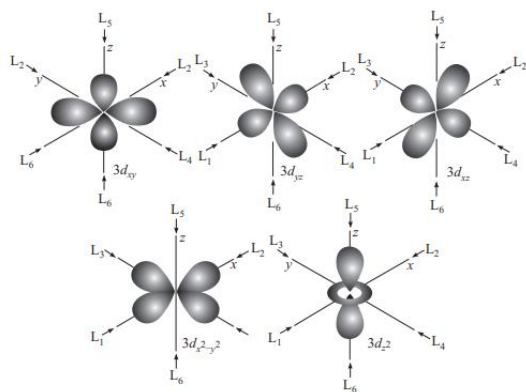


Figure 2: Shapes of d orbitals

In an octahedral complex, six ligands are positioned around a central metal ion in an octahedral geometry. This arrangement maximizes the distance between the ligands to minimize electrostatic repulsion according to VSEPR theory (Valence Shell Electron Pair Repulsion theory). **Anionic Ligands** are often represented as point negative charges in the model. Their negative charge exerts an electrostatic repulsion on the metal ion's d-electrons. **Neutral Ligands** are treated as having a dipole moment. While they don't carry a net charge, the partial negative charge associated with them can also influence the metal ion's d-orbitals. When ligands approach the metal ion along the x, y,

and z axes, they interact most strongly with the d-orbitals that have lobes aligned along these axes.

The three d levels isolated an higher party of double and a inferior get-together of three, the spilling of the levels is kept an eye out for by the image Δ . Expecting we figure the nil of energy as the situation acquire if altogether of the spirit three d orbitals had collaborated similarly through the 6 ligands. It sounds like you're discussing the crystal field splitting in an octahedral field, where the five degenerate 3d orbitals of a transition metal ion are split into two distinct sets of energy levels.

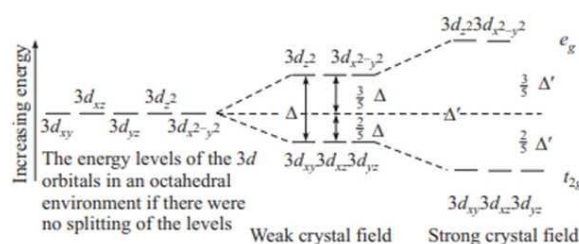


Figure 3: The parting of the 3d levels in an octahedral climate of ligands.

In the incident that we proper presently remember the ex. for alternate steel particle through solitary one three d electron joined octahedrally via using 6 ligands, for example $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$, formerly these solitary three d electron will often coordinate unique of the 3 scalawag decrease levels (t_{2g}). Progress steel particles are disguised when you consider that radioactivity in the plain attain correct rehash to set off this automated alternate, and unequivocally $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ particles are purple for the reason that green light (cross over around 500 nm) is held, as an example white mild brief green light gives pink mild. The association amongst An rehash of bright held is specified by the standard clarifications $\Delta = h\nu$

Where h is Planck's dependable and ν is the rehash accustomed.

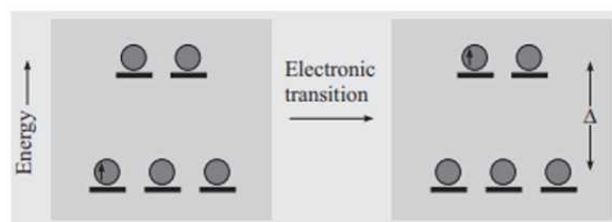


Figure 4: The electronic ironist atom responsible for the conspicuous upkeep in $\text{Ti}(\text{H}_2\text{O})_6^{3+}$. An electron goes through a change from a lower-energy d orbital

to a higher-energy d orbital. The energy change climbs to the crystal field isolating Δ .

Comparable contemplations put on to structures within focal headway metal particle has additional one 3d electrons yet obviously the occurrence of additional one electron in the 3d orbitals prompts minor ensnarements.



wherever the above atoms then unbiased particles are the ligands could encompass the change metal atom.

2. Ligand Field Theory (LFT)

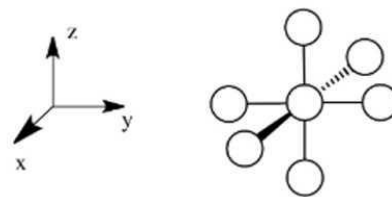
Ligand Field Hypothesis (LFT) for sure assumes a significant part in understanding the reactivity and properties of coordination compounds by looking at how ligand communications impact the metal place's d-orbital energies. Here is a more profound investigate how this hypothesis applies Sub-atomic Orbital (MO) contemplations to coordination chemistry. Ligand Field Hypothesis expands the standards of Atomic Orbital Hypothesis to make sense of what ligand collaborations mean for the energy of metal d-orbitals in coordination compounds. By examining these collaborations, LFT gives experiences into the electronic construction, soundness, reactivity, and spectroscopic properties of metal buildings. This hypothesis helps physicists anticipate and defend the way of behaving of coordination compounds in different synthetic settings.

Ligand Field Hypothesis (LFT) takes on the subsequent point of view, zeroing in on how the collaboration between ligand orbitals and metal d-orbitals influences the in general electronic construction of a coordination complex. By zeroing in on sub-atomic orbital contemplations, Ligand Field Hypothesis gives a more extensive comprehension of how ligands impact the electronic design of metal buildings. This approach considers both the electrostatic repugnance and the holding communications among metal and ligand orbitals, offering bits of knowledge into the soundness, reactivity, variety, and attractive properties of coordination compounds.

Totally! The coordination calculation of ligands around a metal community essentially impacts how the metal's d-electrons collaborate with the ligand's orbitals. This connection influences the energy levels of the d-orbitals in different ways relying upon the calculation of the coordination complex. The math of the coordination complex essentially influences the d-orbital parting and, subsequently, the electronic construction of the metal community.

Octahedral case-

Expect a compound takes an octahedral coordination circle. Recognize the 6 ligands completely invention laterally the x, y and z axes.



Here are d orbitals with the intention to relate unequivocally with these ligands: the $d_{x^2-y^2}$, which

lies it seems that x and y axes, and d_{z^2} , obviously at the z turn.

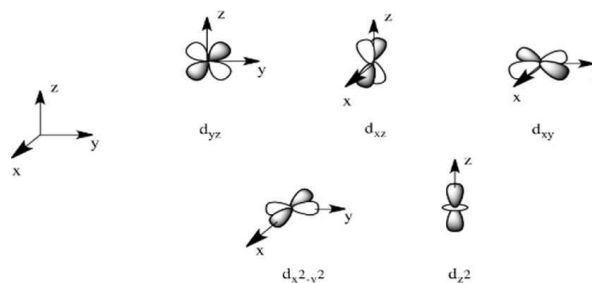
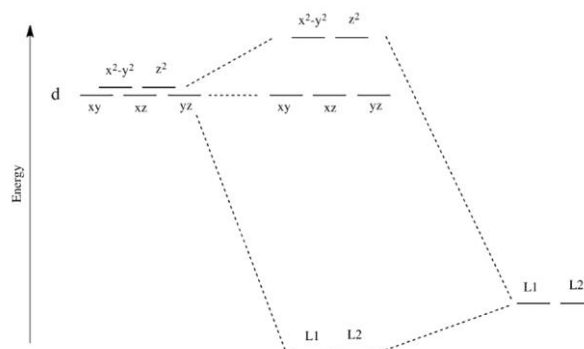


Diagram beneath is easy. The ligands may even engage through "s" and "p" orbitals, then on behalf of instant are not accepted approximately them. We additionally may not fear around communications since the opposite 4 ligands with the "d" orbitals (feasible with the aid of symmetry concerns, but additionally a greater complex photograph).

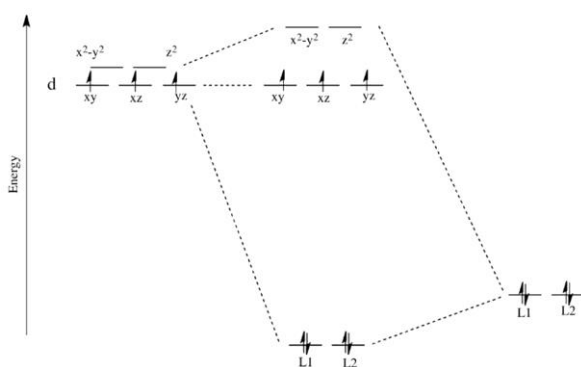


By and by using, evaluate that metals by means of and big have d electrons which might be substantially higher in energy than the ones on commonplace company debris (like oxygen, sulfur, nitrogen or phosphorus). That suggests the antibonding blends might be a ton closer in power to the main d orbitals, considering the way that both are for the most component high in electricity. The holding combo could be a super deal nearer in power to the principle ligand orbitals, in light of the

reality that these ones are through and huge low in strength.

That enthusiastic likeness commonly modifications over into a similarity in shape and location as properly. Thusly, the antibonding combo between a d orbital and a ligand orbital is a ton like the number one d orbital. The maintaining mix is more like the primary ligand orbital than the principle d orbital. Because of these likenesses, inorganic logical professionals each every so often imply the ones antibonding orbitals like they have been at this factor the predominant d orbitals.

These two orbitals will be received usually high up strength by means of sigma conserving courting with the provider orbitals. Expecting that there are electrons within the picture, it is able to appearance some thing like this:



• Acknowledge 6 ligands altogether untruth laterally the x, y and z hatchets.

• The $d_{x^2-y^2}$ and the d_{z^2} orbitals untruth laterally the connection hatchets.

• The 2 orbitals will happen gotten to some degree high up energy.

• These orbitals look like antibonding levels.

• These orbitals are now and again called the "eg" set of orbitals. The term "eg" comes from the study of uniformity.

Of course, the other three d orbitals, the d_{xy} , d_{xz} and d_{yz} .

• The d_{xy} , d_{xz} and d_{yz} orbitals all untruth among the connection hatchets.

• The 3 orbitals will happen altered in energy tad.

• The orbitals remain additional similar non-holding orbitals.

• This orbitals are on occasion entitled the "t_{2g}" set of orbitals.

CONCLUSION

The productive combination of coordination compounds with novel ligands displays the capacity of these ligands to introduce exceptional basic and electronic features. Through careful arrangement and smoothing out of designed conditions, we have made a movement of compounds with undeniable coordination conditions. Among the transcendent homes of coordination compounds are the number and plan of the ligands acquainted with the fundamental metallic atom or particle — that is, the coordination wide assortment and the coordination math, in a steady progression. The coordination scope of a specific now not forever establishment by utilizing the general sizes of the steel particle and the ligands. This surrender absolutely represents the essential impacts of your exploration, centering at the effect of novel ligands on coordination compounds and their thoughts for texture innovation. It in this way makes a way for fate examination headings and features the more noteworthy meaning of the study.

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