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STUDY OF SOME BONDING PARAMETERS OF HYPERSENSITIVE TRANSITION OF SOME PR (III) DOPED SYSTEMS WITH AMIDE CONTAINING LIGANDS AND THEIR ANTIBACTERIAL ACTIVITY

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ABSTRACT

In the present research some bonding parameters of hypersensitive transition of Pr(III) doped systems with three ligands having amide group have been done. For this research we have choose four parameters such as nephelauxetic ratio (β), bonding parameter ($b^{1/2}$), Sinha's covalency parameter (δ%) and covalency angular overlap parameter (η). From the observed data of these parameters, it concludes that in the bonding between Pr(III) ion and amide group of ligands, the involvement of 4f-orbital has very less as compared to transition metals. In the present study we have also investigated the antibacterial activity of various doped systems. This antibacterial activity is investigated against the Escherichia coli and Staphylococcus aureus.

Keywords *– Hypersensitive transition; Bonding parameters; Sinha's covalency parameter; Covalency angular overlap paramete;r; Antibacterial activity.*

1. INTRODUCTION

The intensity of the absorption band in Ln(III) spectra has been studied both theoretically and experimentally. The theory proposed independently by Judd and Ofelt[1-10] has been reasonably successful in accounting for the intensity for most transitions on the basis of crystal-field induced electric dipole transitions between individual Stark components[11].

Most of the sharp lines like 4f↔4f transitions originating within the 4f-configuration of the lanthanide (III) ions are little affected by the environment of the lanthanide ions. Such transitions have been called hypersensitive transitions by Jorgensen and Judd[12]. The oscillator strengths and shapes of the hypersensitive transitions can be used to probe complex formation, coordination geometry, ligand structure and chelate solvent interactions[13]. The bands having oscillator strength ~10^{-5} and found much sensitive to the ligands & solvents are called hypersensitive transitions. Oscillator strength of the hypersensitive transitions exhibits greater variation than the oscillator strength of non hypersensitive transitions[14,15].

In lanthanides transitions involve only a redistribution of electrons within the 4f-orbitals (f↔f transition) are orbitally forbidden by the selection rule. Crystal field effects in lanthanides are virtually insignificant due to 4f-electrons are well shielded from external charge by $5s^2$ and $5p^6$- sub-shells.

In the present research we have select three amide group containing drugs as ligands. These are Salicylamide [$C_6H_7NO_2$], Niacinamide [$C_6H_6N_2O$] and Lidocaine [$C_{14}H_{22}N_2O$] respectively. Some physical properties of these drugs have given in the table 1.

Table 1: Physical properties of various drugs

Drugs	Molecular Weight	Melting Point	Physical State	Solubility
Salicylamide	137.136	140-144^oC	White to pinc Crystalline Powder	Soluble in hot water, alcohol, ether and
Niacinamide	122.13	130-133^oC	White to off white Powder	Soluble in water and alcohol
Lidocaine	234.33	68.5^oC	White Crystalline Powder	Soluble in hot water, alcohol and ether

Salicylamide is used in treating mild to moderate aches and pains associated with headache, muscle and joint soreness, backache, menstrual cramps, colds and flu, sinusitis, toothache, and minor pain from arthritis, and to reduce fever. It may also be used for other conditions as determined by your doctor. Salicylamide is an analgesic and antipyretic combination. It works by blocking substances in the body that cause fever, pain and inflammation.

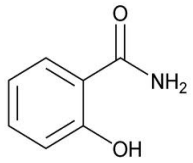


Fig. 1. Chemical Structure of Salicylamide

Niacinamide is a vitamin B-complex supplement. Vitamin B_3 is found in many foods including yeast, meat, fish, milk, eggs, green vegetables, beans and cereal grains. It works by replacing vitamin B_3 in the body. Niacinamide is used for treating or preventing low levels of niacin (vitamin B_3). Niacin is used for high cholesterol. It is also used along with other treatments for circulation problems, migraine headache, dizziness, and to reduce the diarrhea associated with cholera. Niacin is also used for preventing positive urine drug screens in people who take illegal drugs. Niacinamide is used for treating diabetes and two skin conditions called bullous pemphigoid and granuloma annulare.

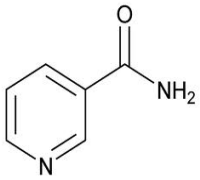


Fig. 2: Chemical Structure of Niacinamide

Lidocaine topical jelly or ointment is used on different parts of the body to cause numbness or loss of feeling for patients having certain medical procedures. It is also used to relieve pain and itching caused by conditions such as sunburn or other minor burns, insect bites or stings, poison ivy, poison oak, poison sumac, minor cuts, or scratches. Lidocaine viscous topical solution is also used to treat sore mouth or throat and also reduce gagging during the taking of X-ray pictures and dental impressions.

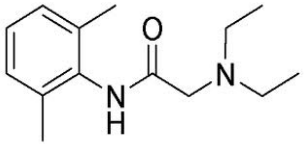


Fig. 3: Chemical Structure of Lidocaine

2. MATERIALS AND METHODS

2.1. MATERIALS

In the present research Salicylamide [$C_6H_7NO_2$], Niacinamide [$C_6H_6N_2O$], Lidocaine [$C_{14}H_{22}N_2O$], ethyl alcohol (C_2H_5OH), distilled water (H_2O) etc. chemicals have been used. All solvents and chemicals used have AR grade. Their purity has checked by thin layer chromatography (TLC). In order to investigate antibacterial activity, disc diffusion method is used. In this method nutrient agar solution, cotton, ethyl alcohol, dilute solutions of various doped systems have been used.

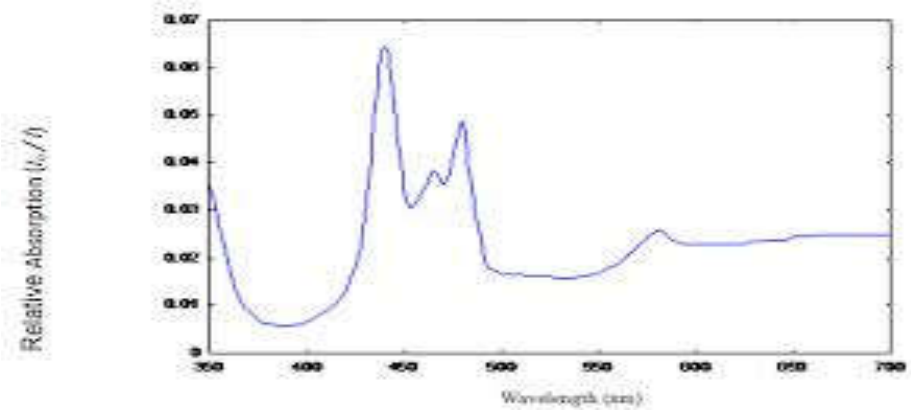
2.1. METHODS

The Pr(III) salt dissolved in suitable amount of ethanol and saturated solutions of various ligands have been prepared in ethanol. In present study three amide ligands has been taken, i.e., Salicylamide [$C_6H_7NO_2$], Niacinamide [$C_6H_6N_2O$] and Lidocaine [$C_{14}H_{22}N_2O$]. Then both solutions have mixed together to form three doped systems. Absorption spectra of doped systems have been recorded at pH-7. For this purpose double beam UV-Visible spectrophotometer has been used. In double beam spectrophotometer, the light ray is divided in to two parts or beams. One beam is passed through the reference material and other beam is passed through the sample. The reference beam intensity is taken as zero absorbance.

The investigation on antimicrobial activity of different types of compounds is not only useful for the development of new drugs but it is also essential to ascertain the toxic nature of the compound. Among various available methods most widely used method consist of determining the antibacterial activity of the concerned compounds by adding it in varying concentration to the culture of test organism. In the present work the biological activity in terms of their growth inhibitory property on specific known bacterial culture against amide group containing drugs and their doped systems with Pr(III) have been evaluated by standard disc diffusion method. The bacterial subculture of Escherichia coli and Staphylococcus aureus has been used as test organism and the sample have been tested against these stains. The study indicates that few of the systems having better antimicrobial activity than ligands.

3. RESULTS AND DISCUSSION

The absorption bands of Pr(III) doped systems appears in the Visible region. The four bands have appear in the visible region. These bands appears due to the transitions from ground levels $^3H_4$ to the excited J-levels, i.e., $^3P_2$, $^3P_1$, $^3P_0$ and $^1D_2$.



In these systems red shift has been observed. This red shift of the bands is due to the expansion of the radius of central metal orbital, resulting the decrease of the inter-electronic repulsion parameters. This phenomenon is called nephelauxetic effect. The very less values of bonding parameter ($b^{1/2}$) suggest that the very less involvement of 4f-orbital[16-30].

The values of various bonding parameters such as nephelauxetic ratio (β), bonding parameter ($b^{1/2}$), Sinha's covalency parameter (δ%) and Covalency angular overlap parameter (η) reveals that the involvement of 4f-orbitals has negligible for lanthanide complexes as compared to transition metals. The relationship among the various parameters has been given as-

$b_{1/2} = [½ (1-\beta)]^{1/2}$

$\delta = [1-\beta / \beta] X 100$

$\eta = [1 - \beta^{1/2} / \beta^{1/2}]$

Where,

β = Nephelauxetic Ratio

$b^{1/2}$ = Bonding Parameter

$\delta\%$ = Sinha's covalency parameter

η = Covalency angular overlap parameter

The values of various bonding parameters have given as-

Table 2: Computed Values of β , $b^{1/2}$, $\delta\%$ and η

Pr(III) Doped system	β	$b^{1/2}$	δ%	η
Pr(III)-Salicylamide	0.99896975	0.022696	0.103131	0.000516
Pr(III)-Niacinamide	0.99807817	0.030999	0.192553	0.000962
Pr(III)-Lidocaine	0.99729717	0.036762	0.271016	0.000516

4. CONCLUSION

Three doped systems of Pr(III) ions with amide ligands in ethanol have been prepared. Solution spectra of each system have been recorded in UV-Visible and Near IR - range. By the investigations of bonding parameters, it has been concluded that the nephelauxetic effect for all doped systems has observed. The values of various parameters such as nephelauxetic ratio (β), bonding parameter ($b^{1/2}$), Sinha's covalency ($\delta\%$) and Covalency angular overlap parameter (η) reveals that the involvement of 4f-orbital has negligible for lanthanide complexes as compared to transition metals. It has also been found that antimicrobial activity of systems has better than ligand solution.

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