JETIR.ORG ISSN: 2349-5162 | ESTD Year : 2014 | Monthly Issue
JOURNAL OF EMERGING TECHNOLOGIES AND INNOVATIVE RESEARCH (JETIR)
An International Scholarly Open Access, Peer-reviewed, Refereed Journal

ELECTRONIC SPECTRAL STUDIES OF DOPED Nd^{3+}ION IN ALCOHOLIC SOLUTION OF ORGANIC OXIMES WITH SPECIAL EMPHASIS ON SYMMETRY CHANGE.

[1]Jaishanker Acharya, [2]Madhusudan Sharma

[1]Associate Professor, [2]Assistant Professor

[1]Department of Chemistry,

[1]Govt. Dunger College, Bikaner-334 003, Rajasthan, India

Abstract : The change in symmetry around (stereo-environment) the doped Nd^{3+} ion in various solutions of some organic oximes has been studied for various electronic spectral parameters. The parameters viz. Slater-Condon (F_K), Racah (E^k), Lande (ζ_{4f}), Judd-Ofelt (T_λ), Intensity of hypersensitive band, bonding parameter for doped in solution of organic oximes have been studied. The study provides useful information about interelectronic repulsion and spin interaction involved in metal-ligand bond.

Keywords : Hypersensitive transition, Doped systems, stereo-environment.

Introduction

Interest of researchers in lanthanoide materials is due to their numerous applications such as scintillators, visible ultraviolet lasers, phosphors for fluorescent lighting and plasma displays, luminescent chemosensors for medical diagnostics, shift reagents for NMR spectroscopy, as well as in various industries and biological studies[1-8].

Electronic spectral studies of lanthanoide ion complexes with reference to Judd-Ofelt parameters have been found to have due significance[9]. This is because of strong validity of the theory given by Judd-Ofelt for intensity of $f-f$ transitions. The various parameters given by Judd-Ofelt have been used to explain covalency and symmetry around lanthanoide ion.

In the present study six organic oximes viz., acetoxime(A), acetophenoneoxime(B), bcnzophenoneoxime(C). diacetylmonooxime(D), cyclooctanoneoxime(E) and -camphoreoxime(F) hve been used as ligands. The solution of each ligand was prepared in 60% aqueous ethanol solution (v/v) and a constant volume of $NdCI_3.6H_20$ salt solution (w/v) has been added to this solution. Nd^{3+} ion has been doped in solutions of these oximes separately in the metal ligand ratio of 1:1 and 1:2.

For Nd^{3+} doped systems, we have observed eleven peaks in the range of 400-900 nm range[10-12]. These peaks are due to $^2P_{1/2}$, $^4G_{11/2}$, $^2G_{9/2}$, $^2K_{15/2}$, $^4G_{9/2}$, $^4G_{7/2}$, $^4G_{5/2}$, $^4F_{9/2}$, $^4F_{7/2}$, $^4F_{5/2}$ and $^4F_{3/2}$ levels. In Nd^{3+} ion doped system, the transition $^4I_{9/2} \rightarrow {}^4G_{5/2}$ is hypersensitive transition.

Results and discussion

The calculation of parameters viz.Slater-Condon (F_K), Racah (E^k), Lande (ζ_{4f}), Oscillator strength (P), Judd-Ofelt (T_λ) have been computed by the programme developed by earlier workers [13- 16].

The computed values of oscillator strength, Judd-Ofelt parameter , energies of various peak, bonding parameters , Slater-Condon (F_K), Lande (ζ_{4f}), Racah (E^k) parameters, nephelauxetic ratio and various other have been tabulated (Tables 1-8).

Spectral intensity parameters

The computed values of oscillator strength (P_{obs} and P_{cal}) for Nd^{3+}-doped systems have been tabulated . The observed values of oscillator strength for $^4G_{5/2}$ band (hypersensitive transition) varies from 1.712×10^{-5} to 2.948×10^{-5}.

The values of T_4/T_6 varies from 0.135 to 0.377. On the basis of values of T_4/T_6 systems can be classified as

(1)CLASS-1. T_4/T_6 values varying in between 0.135 to 0.2103 . ligands were B,C, D,& F with metal-ligand ratio 1:1.

(2) CLASS-2. T_4/T_6 values varying in between 0.2445 to 0.2844 . ligands were B,C,D,&F with metal-ligand ratio 1:2.

(3) CLASS-3. T_4/T_6 values varying in between 0.2994 to 0.3770. ligands were A & E with metal-ligand ratio 1:1 as well as with 1:2 (both).

These three CLASSES (1, 2 & 3) reveal that on changing the metal to ligand ratio for ligands B,C,D & F symmetry around the cation or symmetry of stereo environment around the doped Nd^{3+} ion changes, where as for ligands A and E symmetry remain same.

The values of T_4 / T_2 varies from 0.1194 to 0.6129. On the basis of values of T_4 / T_2 systems can be classified as :-

(1) CLASS-1. T_4/T_2 values varying in between 0.110 to 0.160 . Ligands were D & F with metal-ligand ratio 1 and 1:2, respectively.

(2) CLASS-2. T_4/T_2 values varying in between 0.220 to 0.280 . Ligands were B, C (with metal-ligand ratio 1:1 and 1:2 each) & D with metal-ligand ratio 1:2.

(3) CLASS-3. T_4/T_2 values varying in between 0.340 to 0.350. Ligand was A with metal-ligand ratio 1:1 as well as 1:2.

(4) CLASS-4. T_4/T_2 values varying in between 0..4000 to 0.6200 . Ligands were E (with metal-ligand ratio 1:1 and 1:2 each) & F with metal-ligand ratio 1:1.

In Nd^{3+} doped systems, variation in the coordination number (T_4/T_2) is more than the variation in the symmetry (T_4/T_6) around Nd^{3+} ion.

The value of nephelauxetic ratio (β), for Nd^{3+} doped system varies from 0.9705 to 0.9825. Since the value of β is less than one for all the systems hence presence of covalent character in metal-ligand linkage is proved.

The values of Slater-Condon parameters have been tabulated. The value of F_2 parameter for Nd^{3+} doped systems varies from 321.7 cm^{-1} to 325.7 cm^{-1}. The value of F_4 parameter for Nd^{3+} doped systems varies from 51.97 cm^{-1} to 54.36 cm^{-1}. The value of F_6 parameter for Nd^{3+} doped systems varies from 5.085 cm^{-1} to 5.242 cm^{-1}.

The values of F_2, F_4 and F_6 are slightly lower than corresponding free ion values (F_2 = 331.16 cm^{-1}, F_4 = 50.71 cm^{-1}, F_6 = 5.15 cm^{-1}).

The percentage reduction in F_2 (% r F_2) varies from 1.627% to 2.832% showing very slight decrease in interelectronic repulsions in the Nd^{3+} doped systems.

The Value of F_4/F_2 varies from 0.1602 to 0.1680. These values are nearer to the free ion value (0.1531). The Value of F_6/F_2 varies from 0.0158 to 0.0162. These values are slightly higher than the corresponding free ion value (0.0155).

A small decrease in the value of F_2 parameter, suggest that in Nd^{3+} doped systems, there is a small decrease in interelectronic repulsion between metal ion 4 *f* orbitals and ligand orbitals . This leads to the conclusion that in comparison to transition metal ion having d^n configuration, there is a weak crystal field in the lanthanide complexes or in Ln^{3+} doped systems.

The value of E^1 varies from 5002.84 cm^{-1} to 5081.48 cm^{-1}. The value of E^2 varies from 21.873 cm^{-1} to 22.729 cm^{-1}. The value of E^3 varies from 489.33cm^{-1} to 490.17cm^{-1}. These values of Racah parameters are lower than that of free ion values. These facts also support and indicate, decrease in the interelectronic repulsions, leading to complexation in Nd^{3+} doped systems.

Materials and method :-

All the chemicals and the solvent used were of analytical grade. $NdCI_3.6H_20$ having 99.9% purity was supplied by Indian Rare Earths Ltd. The ligands were dissolved to prepare 0.32 M and 0.16 M solutions in 60% aqueous ethanol (v/v) at room temperature (32 °C). Equal volume (10 ml) of each of these 0.32 M and 0.16 M ligand solution was added in 10 ml solution of 0.16M $NdCI_3.6H_20$ to get systems of having metal to ligand ratio I : 2 and I : I respectively. Solution spectra of these twelve systems were recorded by using standard spectrophotometer (Biomate UV-Visible spectro-photometer v7.07) in the range of 400 to 900 nm.

Table-1. Computed values of oscillator strength for Nd^{3+} doped systems

SN	Levels	Nd^{3+}+solvent		Nd^{3+}+A1		Nd^{3+}+A2		Nd^{3+}+B1		Nd^{3+}+B2		Nd^{3+}+C1		Nd^{3+}+C2	
		P obs	P Cal	P obs	P Cal	Pobs	P obs	P obs	P Cal	P obs	P Cal	Pobs	PCal	P obs	P Cal
1	$^2P_{1/2}$	4.345 X10^{-7}	3.219 X10^{-7}	7.4920 X10^{-7}	3.8931 X10^{-7}	3.9084 X10^{-7}	3.7948 X10^{-7}	9.9744 X10^{-7}	3.5127 X10^{-7}	7.6515 X10^{-7}	2.7953 X10^{-7}	7.2679 X10^{-7}	3.5260 X10^{-7}	6.1520 X10^{-7}	2.581 X10^{-7}
2	$^4G_{11/2}$	5.4362 X10^{-7}	2.8615 X10^{-7}	1.0830 X10^{-6}	3.0370 X10^{-7}	7.0716 X10^{-7}	2.5784 X10^{-7}	1.5737 X10^{-6}	2.9090 X10^{-7}	9.8176 X10^{-7}	2.9496 X10^{-07}	1.0149 X10^{-06}	3.1397 X10^{-7}	1.2686 X10^{-6}	3.051 X10^{-7}
3	$^2G_{9/2}$	4.1104 X10^{-7}	5.473 X10^{-7}	6.3173 X10^{-7}	5.8410 X10^{-7}	3.1625 X10^{-7}	5.0575 X10^{-7}	6.3161 X10^{-7}	1.5521 X10^{-7}	5.8742 X10^{-7}	5.5864 X10^{-07}	5.1606 X10^{-7}	6.0032 X10^{-7}	4.6496 X10^{-7}	5.7118 X10^{-7}
4	$^2K_{15/2}$	4.8918 X10^{-7}	4.6632 X10^{-7}	8.719 X10^{-7}	4.9086 X10^{-7}	5.2106 X10^{-7}	4.1163 X10^{-7}	7.9699 X10^{-7}	5.5423 X10^{-7}	7.1059 X10^{-7}	4.8674 X10^{-07}	7.4150 X10^{-7}	5.1214 X10^{-7}	6.8392 X10^{-7}	5.0665 X10^{-7}
5	$^4G_{9/2}$	1.393 X10^{-6}	1.6737 X10^{-6}	1.7600 X10^{-6}	1.7992 X10^{-6}	1.2165 X10^{-6}	1.5773 X10^{-6}	1.6222 X10^{-6}	1.7274 X10^{-6}	1.5236 X10^{-6}	1.691X 10^{-6}	1.8986 X10^{-6}	1.8347 X10^{-6}	1.5790 X10^{-6}	1.7112 X10^{-6}
6	$^4G_{7/2}$	2.827 X10^{-6}	3.9719 X10^{-6}	3.042 X10^{-6}	4.1711 X10^{-6}	2.4054 X10^{-6}	3.8248 X10^{-6}	2.9647 X10^{-6}	4.1812 X10^{-6}	3.0370 X10^{-6}	3.9992 X10^{-6}	3.1779 X10^{-6}	4.3235 X10^{-6}	2.7514 X10^{-6}	3.8801 X10^{-6}
7	$^4G_{5/2}$	2.431 X10^{-5}	2.4095 X10^{-5}	2.394 X10^{-5}	2.3475 X10^{-5}	2.2788 X10^{-5}	2.2525 X10^{-5}	2.6533 X10^{-5}	2.5831 X10^{5}	2.5560 X10^{-5}	2.4986 X10^{-5}	2.6546 X10^{-5}	2.5904 X10^{-5}	2.3542 X10^{-5}	2.3058 X10^{-5}
8	$^4F_{9/2}$	6.986 X10^{-7}	8.5696 X10^{-7}	1.0755 X10^{-6}	8.9478 X10^{-7}	5.8548 X10^{-7}	7.4786 X10^{-7}	1.1902 X10^{-6}	8.6490 X10^{-7}	1.3714 X10^{-6}	8.9537 X10^{-7}	1.9864 X10^{-6}	9.3914 X10^{-7}	1.2301 X10^{-6}	9.3212 X10^{-7}
9	$^4F_{7/2}$	9.6060 X10^{-6}	8.2261 X10^{-6}	9.997 X10^{-6}	8.5590 X10^{-6}	8.6638 X10^{-06}	7.0857 X10^{-6}	1.0194 X10^{-5}	8.2814 X10^{-6}	1.0579 X10^{-5}	8.6658 X10^{-6}	1.0737 X10^{-5}	9.0259 X10^{-6}	1.0652 X10^{-05}	9.0805 X10^{-6}
10	$^4F_{5/2}$	6.8445 X10^{-6}	8.0747 X10^{-6}	7.6274 X10^{-6}	8.5412 X10^{-6}	5.8359 X10^{-6}	7.2277 X10^{-6}	7.1074 X10^{-6}	8.1924 X10^{-6}	7.0455 X10^{-6}	8.3286 X10^{-6}	7.8420 X10^{-6}	8.8471 X10^{-6}	7.5912 X10^{-6}	8.635 X10^{-6}
11	$^4F_{3/2}$	3.557 X10^{-6}	1.8494 X10^{-6}	3.9246 X10^{-6}	2.0795 X10^{-6}	3.8927 X10^{-6}	1.8877 X10^{-6}	4.3499 X10^{-6}	1.9361 X10^{-6}	4.0676 X10^{-6}	1.7696 X10^{-6}	4.2416 X10^{-6}	2.0240 X10^{-6}	3.7438 X10^{-6}	1.754 X10^{-6}
12	rms→ deviations	σ=±8.470X10^{-7}		σ =±8.905X10^{-7}		σ = ±9.9717X10^{-7}		σ = ±1.1716X10^{-6}		σ = ± 1.081X10^{-6}		σ =±1.0605X10^{-6}		σ =± 9.643X10^{-7}	

Table-2. Computed values of oscillator strength for Nd^{3+} doped systems-

SN	Levels	Nd^{3+}+D1		Nd^{3+}+D2		Nd^{3+}+E1		Nd^{3+}+E2		Nd^{3+}+F1		Nd^{3+}+F2	
		Pobs	P Cal	Pobs	P Cal	P Cal	P obs	P Cal	P Cal	P obs	P Cal	P obs	P Cal
1	$^2P_{1/2}$	8.99357 X10^{-7}	2.10589 X10^{-7}	1.0757 X10^{-6}	1.81614 X10^{-7}	8.3421 X10^{-7}	5.00113 X10^{-7}	6.164 X10^{-7}	4.20819 X10^{-7}	6.9607 X10^{-7}	1.98336 X10^{-7}	6.10995 X10^{-7}	3.40145 X10^{-7}
2	$^4G_{11/2}$	1.15611 X10^{-6}	1.95197 X10^{-7}	1.30063 X10^{-6}	2.85593 X10^{-7}	2.29793 X10^{-6}	3.22395 X10^{-7}	7.2703 X10^{-7}	3.22149 X10^{-7}	9.3909 X10^{-7}	2.8126 X10^{-7}	8.13272 X10^{-7}	2.77865 X10^{-7}
3	$^2G_{9/2}$	4.26751 X10^{-7}	3.75552 X10^{-7}	6.54841 X10^{-7}	5.37041 X10^{-7}	1.24373 X10^{-6}	6.23647 X10^{-7}	4.43974 X10^{-7}	6.09849 X10^{-7}	5.3587 X10^{-7}	5.25428 X10^{-7}	4.89687 X10^{-7}	5.28451 X10^{-7}
4	$^2K_{15/2}$	6.41853 X10^{-7}	3.19328 X10^{-7}	8.15327 X10^{-7}	4.79882 X10^{-7}	8.87168 X10^{-7}	5.11266 X10^{-7}	8.9815 X10^{-7}	5.18595 X10^{-7}	6.4670 X10^{-7}	4.70153 X10^{-7}	8.96379 X10^{-7}	4.50449 X10^{-7}
5	$^4G_{9/2}$	1.13987 X10^{-6}	1.14702 X10^{-6}	1.78508 X10^{-6}	1.59978 X10^{-6}	2.69689 X10^{-6}	1.93645 X10^{-6}	1.91506 X10^{-6}	1.86884 X10^{-6}	1.5172 X10^{-6}	1.56798 X10^{-6}	1.71796 X10^{-6}	1.61937 X10^{-6}
6	$^4G_{7/2}$	2.61673 X10^{-6}	2.82076 X10^{-6}	2.99999 X10^{-6}	3.99213 X10^{-6}	4.75757 X10^{-6}	4.20059 X10^{-6}	4.05769 X10^{-6}	3.88995 X10^{-6}	3.0123 X10^{-6}	3.71898 X10^{-6}	3.66147 X10^{-6}	3.55896 X10^{-6}
7	$^4G_{5/2}$	1.88205 X10^{-5}	1.83551 X10^{-5}	2.9485 X10^{-5}	2.87134 X10^{-5}	1.96627 X10^{-5}	1.89559 X10^{-5}	1.71283 X10^{-5}	1.68087 X10^{-5}	2.4969 X10^{-5}	2.45766 X10^{-5}	1.84089 X10^{-5}	1.80499 X10^{-5}
8	$^4F_{9/2}$	7.47286 X10^{-7}	5.89176 X10^{-7}	1.73248 X10^{-6}	8.94547 X10^{-7}	9.92924 X10^{-7}	9.25132 X10^{-7}	8.27498 X10^{-7}	9.37848 X10^{-7}	8.0432 X10^{-7}	8.72342 X10^{-7}	8.31811 X10^{-7}	8.2024 X10^{-7}
9	$^4F_{7/2}$	6.79768 X10^{-6}	5.65054 X10^{-6}	1.05775 X10^{-5}	8.71586 X10^{-6}	1.00382 X10^{-5}	8.79881 X10^{-6}	1.03796 X10^{-5}	9.03803 X10^{-6}	9.9529 X10^{-6}	8.50772 X10^{-6}	9.04675 X10^{-6}	7.89675 X10^{-6}
10	$^4F_{5/2}$	4.97025 X10^{-6}	5.50871 X10^{-6}	7.1701 X10^{-6}	8.10512 X10^{-6}	8.82538 X10^{-6}	9.06231 X10^{-6}	8.09124 X10^{-6}	9.06069 X10^{-6}	6.9665 X10^{-6}	7.96793 X10^{-6}	7.13953 X10^{-6}	7.83964 X10^{-6}
11	$^4F_{3/2}$	2.51261 X10^{-6}	1.23644 X10^{-6}	3.78852 X10^{-6}	1.4915 X10^{-6}	3.63807 X10^{-6}	2.43163 X10^{-6}	3.54489 X10^{-6}	2.2282 X10^{-6}	3.1842 X10^{-6}	1.51691 X10^{-6}	3.03632 X10^{-6}	1.86788 X10^{-6}
12	rms→deviations	σ = ± 6.75697X10^{-7}		σ =± 1.12364X10^{-6}		σ = ± 9.03553X10^{-7}		σ = ±6.7365X10^{-7}		σ = ± 8.1153X10^{-7}		σ = ± 5.944X10^{-7}	

Table-3. Energies of various bands for Nd^{3+} doped systems-

SN	Levels	Nd^{3+}+ solvent		Nd^{3+}+A1		Nd^{3+}+A2		Nd^{3+}+B1		Nd^{3+} +B2		Nd^{3+}+ C1		Nd^{3+}+C2	
		E obs (cm^{-1})	E cal (cm^{-1})	E obs (cm^{-1})	E cal (cm^{-1})	Eobs (cm^{-1})	E cal (cm^{-1})	Eobs (cm^{-1})	Ecal (cm^{-1})	E obs (cm^{-1})	E cal (cm^{-1})	E obs (cm^{-1})	E cal (cm^{-1})	E obs (cm^{-1})	E cal (cm^{-1})
1	$^2P_{1/2}$	23291	23102.7	23290.4	23098.2	23290.2	23097.8	23290.9	23091.1	23299.4	23102.7	23291	23094.7	23289.9	23080.3
2	$^4G_{11/2}$	21641	21398.6	21619.1	21347.4	21635.6	21331.2	21619.2	21330.5	21619.8	21306.8	21629.2	21350.7	21606	21308.8
3	$^2G_{9/2}$	21236	21212.9	21230.0	21219.9	21261.0	21244.2	21241.7	21227.9	21230.3	21228.8	21240.9	21228.2	21249.9	21232.5
4	$^2K_{15/2}$	20945	21156.8	20953.5	21184.7	20959.8	21212.0	20952.4	21195.0	20959.9	21213.0	20951.5	21186.8	20949.4	21203.8
5	$^4G_{9/2}$	19499	19504.6	19498.5	19486.2	19508.6	19485.7	19494.7	19479.7	19505.1	19471.4	19507.4	19486.5	19495.9	19472.3
6	$^4G_{7/2}$	19066	19192.6	19064.1	19192.8	19079.3	19199.5	19064.8	19190.7	19073.5	19192.6	19068.2	19189.7	19058.8	19190.5
7	$^4G_{5/2}$	17144	17155.5	17165.3	17139.5	17136.3	17124.9	17140.1	17125.0	17138.4	17123.6	17128.9	17127.1	17134.9	17116
8	$^4F_{9/2}$	14612	14676.8	14594.6	14649.9	14580.3	14646.7	14576.5	14643.2	14565.3	14630.5	14591.8	14655.3	14562.8	14631.8
9	$^4F_{7/2}$	13337	13203.4	13325.2	13173.7	13324.3	13161.5	13329.2	13161.9	13319.1	13149.9	13327.0	13173.0	13321.7	13148.5
10	$^4F_{5/2}$	12459	12385.0	12434.2	12360.1	12432.0	12348.4	12435.3	12348.9	12425.4	12339.4	12435.7	12357.5	12432.2	12337.6
11	$^4F_{3/2}$	11513	11383.1	11487.8	11370.4	11489.1	11360.1	11479.2	11360.5	11471.3	11358.9	11487.5	11363.1	11477.2	11353.3
12	rms → σ (cm^{-1}) deviations	±135.05		±143.5		±154.7		±151.6		±156.4		±146.5		±158.00	

Table-4. Energies of various bands for Nd^{3+} doped system-

SN	Level	Nd^{3+}+D1		Nd^{3+}+D2		Nd^{3+}+E1		Nd^{3+}+E2		Nd^{3+}+F1		Nd^{3+}+F2	
		Eobs (cm^{-1})	E cal (cm^{-1})	Eobs (cm^{-1})	E cal (cm^{-1})	E obs (cm^{-1})	E cal (cm^{-1})	E obs (cm^{-1})	E cal (cm^{-1})	E obs (cm^{-1})	E cal (cm^{-1})	E obs (cm^{-1})	E cal (cm^{-1})
1	$^2E_{1/2}$	23282.28	23098.6	23282.2	23083.6	23280.2	22976.8	23247.7	22943.6	23291.2	23078.2	23187.9	22951.8
2	$^4G_{11/2}$	21629.27	21374.8	21629.2	21324	21561	21430	21584.3	21348	21635.7	21349	21591.4	21368.6
3	$^2G_{9/2}$	21256.74	21236.7	21256.7	21238.1	21227.8	21161.8	21213.2	21167.6	21236.1	21217.6	21221.2	21206
4	$^2K_{15/2}$	20956.3	21183.9	20956.3	21203.3	20847.3	21032.2	20868.3	21067.4	20940.4	21171.7	20919.8	21091.9
5	$^4G_{9/2}$	19497.8	19497.5	19497.8	19480.6	19451.7	19488.9	19487.7	19474.2	19506.9	19484.8	19515	19489.6
6	$^4G_{7/2}$	19061.6	19192.5	19061.6	19194.9	19010.3	19140.7	19042.1	19165.6	19063.6	19187.9	19058	19175.2
7	$^4G_{5/2}$	17161.26	17128.4	17145.0	17120.8	17096	17116.8	17147	17135.9	17146	17132.9	17081.6	17120.1
8	$^4F_{9/2}$	14615.19	14670.9	14570.1	14641	14612	14684.0	14548.2	14629.6	14574.6	14650.1	14590.7	14651.3
9	$^4F_{7/2}$	13342.12	13185.3	13327.4	13156.9	13330.3	13211.8	13296.3	13169.6	13327.4	13172.8	13333.3	13175.9
10	$^4F_{5/2}$	12443.64	12366.8	12436.1	12344.6	12445.9	12387.3	12427.7	12360.0	12433.6	12358.7	12453.1	12361.8
11	$^4F_{3/2}$	11482.35	11365.2	11479.0	11356.8	11500.7	11358.1	11482	11361.4	11477	11365.7	11490.7	11352.8
12	rms → σ (cm^{-1})	±140.17539		±156.67819		±138.0242		±149.9613		±149.3		±137.1	

Table-5. Computed values of Slater Condon parameters for Nd^{3+} doped systems-

SN	SYSTEMS	M : L	F_2 (cm^{-1})	F_4(cm^{-1})	F_6(cm^{-1})	F_4/F_2	F_6/F_2	% rF_2
1	Nd^{3+} + Solvent	-	325.77	53.05	5.237	0.1628	0.0161	1.6276
2	Nd^{3+} + A1	1:2	324.77	53.78	5.234	0.1656	0.0161	1.9296
3	Nd^{3+} + A2	1:1	323.97	54.2	5.23	0.1673	0.0161	2.1712
4	Nd^{3+} + B1	1:2	324.19	54.02	5.23	0.1666	0.0161	2.1047
5	Nd^{3+} + B2	1:1	324.12	54.34	5.242	0.1677	0.0162	2.1259
6	Nd^{3+} + C1	1:2	324.56	53.72	5.235	0.1655	0.0161	1.9930
7	Nd^{3+} + C2	1:1	323.51	54.36	5.219	0.1680	0.0161	2.3101
8	Nd^{3+} + D1	1:2	324.81	53.47	5.237	0.1646	0.0161	1.9175
9	Nd^{3+} + D2	1:1	323.67	54.24	5.219	0.1676	0.0161	2.2617
10	Nd^{3+} + E1	1:2	324.4	51.97	5.151	0.1602	0.0159	2.0413
11	Nd^{3+} + E2	1:1	322.16	53.64	5.085	0.1665	0.0158	2.7177
12	Nd^{3+} + F1	1:2	324.36	53.73	5.217	0.1656	0.0161	2.0534
13	Nd^{3+} + F2	1:1	321.78	53.64	5.089	0.1667	0.0158	2.8325
14	Nd^{3+} (free ion)	_	331.16	50.71	5.15	0.1531	0.0156	0.0000

Table-6. Computed values of Racah and Lande parameters for Nd^{3+} doped system-

SN	SYSTEMS	M : L	E^1 (cm^{-1})	E^2 (cm^{-1})	E^3 (cm^{-1})	ζ_{4f}	% $r\zeta_{4f}$
1	Nd^{3+} + Solvent	-	5060.5379	22.586	490.1736	853.41	3.460407
2	Nd^{3+} + A1	1:2	5070.7221	22.230	490.0799	845.09	4.401584
3	Nd^{3+} + A2	1:1	5074.2750	21.997	489.7257	843.80	4.547511
4	Nd^{3+} + B1	1:2	5071.5020	22.082	489.7063	844.01	4.523756
5	Nd^{3+} + B2	1:1	5081.4874	21.978	489.8776	839.15	5.073529
6	Nd^{3+} + C1	1:2	5067.8503	22.227	489.5826	848.07	4.06448
7	Nd^{3+} + C2	1:1	5072.4873	21.885	489.5891	840.85	4.881222
8	Nd^{3+} + D1	1:2	5063.6137	22.341	489.4096	852.92	3.515837
9	Nd^{3+} + D2	1:1	5070.5020	21.941	489.6401	843.08	4.628959
10	Nd^{3+} + E1	1:2	5002.8402	22.729	488.3383	868.51	1.752262
11	Nd^{3+} + E2	1:1	5013.6101	21.873	489.9568	846.21	4.274887
12	Nd^{3+} + F1	1:2	5062.5469	22.187	489.8163	846.71	4.218326
13	Nd^{3+} + F2	1:1	5060.5379	22.586	490.1736	853.41	3.515837

Table-7. Computed values of Judd-Ofelt parameters for Nd^{3+} doped system.

SN	System	M:L	T_2	T_4	T_6	T_4/T_6	T_4/T_2
1	Nd^{3+} +solvent	-	$1.3X10^{-9}$	$3.6X10^{-10}$	$1.41X10^{-9}$	0.2567	0.2695
2	Nd^{3+}+A1	1:2	$1.2X10^{-9}$	$4.39X10^{-10}$	$1.47X10^{-9}$	0.2994	0.3463
3	Nd^{3+}+A2	1:1	$1.22X10^{-9}$	$4.28X10^{-10}$	$1.21X10^{-9}$	0.3545	0.3497
4	Nd^{3+}+B1	1:2	$1.4X10^{-9}$	$3.96X10^{-10}$	$1.42X10^{-9}$	0.2788	0.2742
5	Nd^{3+} B2	1:1	$1.42X10^{-9}$	$3.15X10^{-10}$	$1.50X10^{-9}$	0.2104	0.2213
6	Nd^{3+}+C1	1:2	$1.44X10^{-9}$	$3.97X10^{-10}$	$1.55X10^{-9}$	0.2561	0.2752
7	Nd^{3+}+C2	1:1	$1.31X10^{-9}$	$2.91X10^{-10}$	$1.57X10^{-9}$	0.1850	0.2228
8	Nd^{3+} D1	1:2	$1.05X10^{-9}$	$2.37X10^{-10}$	$9.71X10^{-10}$	0.2445	0.2270
9	Nd^{3+}+D2	1:1	$1.71X10^{-9}$	$2.05X10^{-10}$	$1.51X10^{-9}$	0.1352	0.1194
10	Nd^{3+}+E1	1:2	$9.20X10^{-10}$	$5.64X10^{-10}$	$1.50X10^{-9}$	0.3770	0.6129
11	Nd^{3+}+E2	1:1	$8.15X10^{-10}$	$4.75X10^{-10}$	$1.55X10^{-9}$	0.3063	0.5830
12	Nd^{3+}+F1	1:2	$1.44X10^{-9}$	$2.24X10^{-10}$	$1.48X10^{-9}$	0.1513	0.1554
13	Nd^{3+}+F2	1:1	$9.49X10^{-10}$	$3.85X10^{-10}$	$1.35X10^{-9}$	0.2844	0.4057

Table-8. Computed values of bonding parameters for Nd^{3+}doped systems-

SN	Systems	M:L	β	$b^{1/2}$	δ %	η
1	Nd^{3+} + Solvent	-	0.9825	0.0935	1.78117	$8.87X10^{-3}$
2	Nd^{3+} +A1	1:2	0.9795	0.1012	2.09290	$1.04X10^{-2}$
3	Nd^{3+} +A2	1:1	0.9771	0.1070	2.34367	$1.17X10^{-2}$
4	Nd^{3+} +B1	1:2	0.9778	0.1055	2.27040	$1.13X10^{-2}$
5	Nd^{3+} +B2	1:1	0.9775	0.1060	2.30179	$1.14X10^{-2}$
6	Nd^{3+} +C1	1:2	0.9789	0.1028	2.15548	$1.07X10^{-2}$
7	Nd^{3+} +C2	1:1	0.9757	0.1102	2.49052	$1.24X10^{-2}$
8	Nd^{3+} +D1	1:2	0.9796	0.1010	2.08248	$1.04X10^{-2}$
9	Nd^{3+} +D2	1:1	0.9762	0.1091	2.43802	$1.21X10^{-2}$
10	Nd^{3+} +E1	1:2	0.9784	0.1040	2.20768	$1.10X10^{-2}$
11	Nd^{3+} +E2	1:1	0.9716	0.1191	2.92301	$1.45X10^{-2}$
12	Nd^{3+} +F1	1:2	0.9783	0.1042	2.21813	$1.10X10^{-2}$
13	Nd^{3+} +F2	1:1	0.9705	0.1215	3.03966	$1.51X10^{-2}$

Acknowledgement

The authors are thankful to Dr. G.P.Singh. Principal. Dunger College ,Dr.Raja Ram, Assitant professor,DCB,Bikaner and Head, Department of Chemistry for providing research facilities. Author (Jaishanker Acharya) is highly thankful to UGC,CRO (Bhopal) for granting minor research project.

References

[1] Anees A.Ansari, Aslam Khan, Manawwer Alam, Masood A.Siddiqui, Naushad Ahamad, Abdulaziz A.Alkhedhairy, *Collids and Surfaces B: Biointerfaces* ,2020, **189,** 110877.
[2] Y. K. Sharma, S. S. L. Surana, C. L. Gehlot and S. P. Tandon, *Indian J. Eng. & Mater. Sci* .. 2003, **10**, 216.
[3] V. K. Gupta, S. Jain and S. Chandra, *Anal. Chim. Acta*, 2003, **486**, 199.
[4] A. Rai and V. K. Rai, *J. Indian Chem. Soc.*, 2005, **82**, 698.
[5] J.-C. G. Bunzli and C. Piguet, *Chem. Rev., 2002*, **102**, 1897.
[6] G P. Mines, *J. Physiol. London*, 1910, **40**, 327.
[7] J. Y. Lettvin, W. F. Pickard, W. S. McCulloch and W. Pitts, *Nature*, 1964, **202**, 1338.
[8] J.-C. G. Bunzli. *Acc. Chem. Res.*, 2006, **39,** 53.
[9] M.P. Gautum, Ashok Yadav and S. N. Limaye, Asian J. Chem., 1998, **10**, 415.
[10] B. R. Judd and C. K. Jorgensen, *Mol. Phys.*, 1964, **8**, 281.
[11] W. T. Carnell, *J. Chem. Phys.*, 1965, **42**, 3797.
[12] S. P. Sinha, ·*Spectrochim. Acta*. 1966**, 22**, S7.
[13] (Ms.) Daya Balani and G K. Joshi, *Asian j. Chem.*, 1994, **6,** 801.
[14] (Ms). Aryamitra Pandey, K. P. Soni and G. K. Joshi, *Asian J. Chem.*, .2000, **12**, SIS.
[15] R. D. Peacock, *"Structure and Bonding", Springer-Verlag, Berlin·Heidbelerg*-New York, 1975, **22**, 88.
[16] R. S.Verma, Rama Gupta and G K. Joshi, *I. Indian Chem. Soc:. 2*002, **79**, 802.