2024
11(1), 953

Journal of
MATERIALS NANOSCIENCE

Effect of Co-doped alkali earth metals Ca^{2+}, Mg^{2+}, Sr^{2+} ions on the spectral parameter for rare earth, Pr(III)-2-Amino Benzothiazole doped system in the micellar medium

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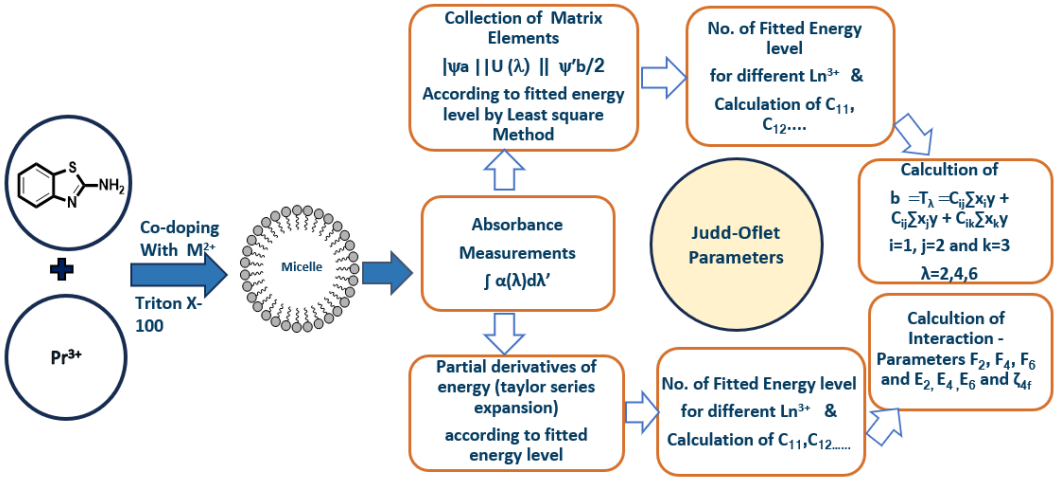
Submitted on: 02-Aug-2024, Accepted and Published on: 12-Sep-2024

Article

ABSTRACT

Electronic transition levels of Pr(III) lanthanide ion with an aromatic heterocyclic ligand containing N, S, and O atom i.e. Pr(III)-2AB system/complex have been determined by electronic spectra in micellar (TX-100) medium at 25°. Using the Gaussian curve, the half band ($\upsilon_{1/2}$) width and energy expression have been determined, such as Taylor's series expansion is utilized to express the j^{th} level's energy. The interactions between lanthanide (III) ion and ligand have been evaluated in terms of Slater-Condon (F_K), Racah (E^K), Lande (ζ_{4f}) parameters, and bonding parameters. Four assignments $^3H_4 \rightarrow {}^3P_2$, $^3H_4 \rightarrow {}^3P_1$, $^3H_4 \rightarrow {}^3P_0$, and $^3H_4 \rightarrow {}^1D_2$ were made to justify these interaction parameters. In this research paper, we have explored theoretical as well as practical analysis of electronic spectra of Pr(III) ion in the micellar medium. The results of interaction parameters have been obtained as F_2=307.10, F_4=76.12, F_6=6.78, E^1=4508.84, E^2=23.58, E^3 =455.88, and ζ_{4f} =761.29.



Keywords: Transition level, Interaction-parameters, Electronic-absorption spectra, and aromatic heterocyclic ligand

INTRODUCTION

Micelles are organized assemblies of amphiphile molecules that have been used extensively as membrane imitates to identify the membrane proteins, and peptides as well as to deliver drugs.[1] They enhance the reaction rate by organizing the reactants on a molecular scale, so it is advantageous to study chemical reactions in an organized system. It provides a better medium for the aggregation of metal ions and ligands. Energy absorption and electronic transition on the interaction of lanthanide ions with organic heterocyclic ligands in the micellar medium has built an understanding of the nature and reactivity of the metal ligand bond. When a photon of light (hυ) is absorbed by a particle, energy is supplied to an electron that can "jump" to an orbital with high energy. The energy absorption is advanced by "operators" related to the frequency of light. The different operators are electric dipole (E.D.) for odd-parity ($P^{\wedge}$), the magnetic dipole (M.D.) for even-parity ($M^{\wedge}$), and the electric quadrupole (E.Q.) operator ($Q^{\wedge}$). Lanthanide ions involve following electronic transitions viz-(i). Sharp absorption band due to intra-configurational 4f→4f transitions (ii). Broader absorption band due to 4f→5d transitions (iii). Broad absorption transition bands due to charge-transfer (M→L) MLCT, (L→M), LMCT, first and second f-f transitions, and 4f→5d transitions are forbidden by the ED. However, non-centrosymmetric interaction allows the mixing the electronic state of opposite parity of 4f wave functions, when a ligand field is acting on the lanthanide

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DOI:10.62110/sciencein.jmns.2024.v11.953
URN:NBN:sciencein.jmns.2024.v11.953
 http://pubs.thesciencein.org/jmns

(III) ion. As a result, the selection rules are relaxed, making the transition partially permitted, which is known as an induced electronic dipole transition (EDT). However, there is no restriction on magnetic dipole transitions (MDT).

Judd-Ofelt Theory (JOT) gives a simple model for f→f transitions in the solid or solution states. After the publication of Judd-Oflet theory[2,3] the value of different parameters like intensity, interaction, and bonding (σ) parameters were computed with absorption maxima of various UV-Visible spectra (Fig.1) of lanthanide system.[4–6] Sharp absorption band due to intra configurationally 4f-4f transitions occur during absorption of UV-Visible radiation. When there is electrostatic interaction, and magnetic interaction between 4f-electrons the transition occurs due to interaction between 4f-electrons of lanthanides, which can be calculated in terms of Slater-Condon (F_K), Lande (ζ_{4f}), and Racah (E^K) parameters. Racah introduced a Taylor series expansion to solve energy levels[7–9] for 4f-4f transitions of rare-earth lanthanide metal complexes in UV-visible region, which have been used by various researchers.[10–19] In order to analyze the inner structure of Ln(III) complexes, it is necessary to examine the 4f-4f transition. Spectra were recorded in the micellar medium for Pr(III)-2AB systems, and ligand including S, O, and N donors atoms which were examined.[20,21] The term "co-doping," is short for "concurrent doping," and describes the deliberate insertion of two distinct dopant components into a substance. Dopants are atoms or ions introduced to a crystalline structure to change its optical properties, magnetic behavior, or electrical conductivity, among other attributes. In this paper, absorption spectra of Praseodymium complexes are studied (Fig.1). The fitted transition levels of Pr(III) lanthanide system can be explained by the following parameters (F_2, F_4, F_6), Lande's (E^K), Racah (ζ_{4f}), Bonding parameter ($b^{1/2}$), Nephelauxetic ratio (β), Sinha's covalency parameters (δ%), Covalency angular overlap parameter (η), and Thermodynamic parameters.[22–24]

Materials and Methods

Pr(III) chloride and 2-Amino benzothiazole were purchased from Sigma-Aldrich. The solvents used to prepare the doped system were of AR grade. Et-OH (99.9%) and Triton-X-100 (100 CMC solutions) were purchased from Jiangsu-Hliaxi International Trade Co. Ltd. In this study Pr(III) ion has been doped with the 0.01M solution of 2-Amino benzothiazole in micellar (Non-ionic) medium and co-doped with alkali earth metal Ca^{2+}, Mg^{2+}, Sr^{2+} ions. The solutions of derivative Benzothiazole have been prepared in Triton X-100 (CMC: 1.8 x 10^{-2} M). The solution spectra (Fig.1) of the system at -25degree centimeters in a 1:3 ratio (Metal: Ligand) has been recorded by using Shimadzu 1800 UV-visible double-beam spectrophotometer with high resolution at ARSD College University of Delhi. Orbital Interactions have been expressed as Slater-Condon (F_K), Lande (ζ_{4f}), and Racah (E^K) parameters.

Slater-Condon and Lande Equation

The Slater-Condon (F_K), K=2,4,6, and Lande's parameter or Spin-Orbit Coupling Constant (ζ_{4f}) were determined using energy expression for j^{th} electronic energy level.[7–9] In the first-order approximation the energy E_j of a j^{th}-level can be expressed by the equation (5).

$$E_j(F_k, \zeta_{4f}) = E_{oj}(F^o_k, \zeta^o_{4f}) + \sum (\partial E_j / \partial F_k)\Delta F_k + (\partial E_j / \partial \zeta_{4f})\Delta\zeta_{4f} \quad \text{----------(5)}$$

k =2, 4, 6

$$E_{obs} = E_{oj} + (\partial E_j/\partial F_2)\Delta F_2 + (\partial E_j/\partial F_4)\Delta F_4 + (\partial E_j/\partial F_6)\Delta F_6 + (\partial E_j/\partial\zeta_{4f})\Delta\zeta_{4f} \quad \text{-------(6)}$$

$$E_{obs} - E_{oj} = (\partial E_j/\partial F_2)\Delta F_2 + (\partial E_j/\partial F_4)\Delta F_4 + (\partial E_j/\partial F_6)\Delta F_6 + (\partial E_j/\partial\zeta_{4f})\Delta\zeta_{4f} \quad \text{------(7)}$$

$$[(E_{obs} - E_{oj}) \div (\partial E_j/\partial F_2)] = \Delta F_2 + [(\partial E_j/\partial F_4) \div (\partial E_j/\partial F_2)]\Delta F_4 + [(\partial E_j/\partial F_6) \div (\partial E_j/\partial F_2)]\Delta F_6 + [(\partial E_j/\partial\zeta_{4f}) \div (\partial E_j/\partial F_2)]\Delta\zeta_{4f} \quad \text{------ (8)}$$

Where,

E_{oj} = Energy of j^{th} level as Zero-order

E_j = Energy of j^{th} level

$\Delta\zeta_{4f}$ = Small deviation in the Lande parameters

ΔF_k =Small deviation in the Slater-Condon parameters

$(\partial E_j / \partial F_k)$ = Partial derivative with respect to F_k

$(\partial E_j / \partial \zeta_{4f})$ = Partial derivative with respect to ζ_{4f}

The values of ΔF_k and $\Delta\zeta_{4f}$ may be evaluated using observed energy values (E_j), reported results of zero-order energies (E_{oj}), partial derivatives ($\partial E_j / \partial F_k$), and ($\partial E_j / \partial \zeta_{4f}$) by partial - multiple regression method.[6,25,26]

The result of Slater-Condon parameters ($F_{k=2,4,6}$), and Lande para-meters (ζ_{4f}) were calculated by equations-

$$F_k = F^o_k + \Delta F_k \text{----------(9)}$$

$$\zeta_{4f} = \zeta^o_{4f} + \Delta\zeta_{4f} \text{----------(10)}$$

Where, $\Delta F_k << F^o_k$, $\Delta\zeta_{4f} << \zeta^o_{4f}$, F^o_k, and ζ^o_{4f} are the zero-order values by Wong.[7]

Racah Parameters or Energy parameters (E^1, E^2, and E^3)

In this case, it is assumed that wave functions are hydrogenic since $E^{K'}$s (Racah parameters) are the linear combination of $F_{K=2,4,6}$ that's why the Racah Parameters can be calculated for Pr(III)-system[27,28] by using the following equations 11-13.

$$E^1 = 14.6818\ F_2 \text{----------(11)}$$

$$E^2 = 0.0768\ F_2 \text{----------(12)}$$

$$E^3 = 1.4844\ F_2 \text{----------(13)}$$

R.M.S. deviations (Energy)

The validity of the parameters, and the deviation were obtained by the root mean square method, and the quality of the fitting by the root means square deviation (R.M.S). The value of R.M.S. is in the typical error range of the Judd-Ofelt fitting which indicates good agreements between the experimental and calculated results. For comparison between calculated (E_{cal}) and observed (E_{obs}) values of energy, the value/data of R.M.S. deviations (σ) by using the relations.

$$\sigma = \{\Sigma (E_{cal}-E_{obs})/N\}^{1/2} \text{----------(14)}$$

Where, N = 4, the number of transition level fitted

Bonding parameters

In bonding parameters, (i) the Nephelauxetic ratio (β), (ii) bonding parameters ($b^{1/2}$), (iii) Covalency angular overlap parameter (η), and (iv) Sinha's covalency parameter (δ%) are included. The complex formation of a free metal ion with ligand

leads to a decrease in the interelectronic repulsion parameter, hence a bathochromic shift of the electronic transition is observed. Jorgensen named this phenomenon the "Nephelauxetic Effect" (β) which means "Cloud expansion effect" in Greek. The value of bonding parameter (β) near 1.0 reflects the decrease in the percentage of covalency in the solution state, which is thermodynamically less stable, confirming the interaction between Ln(III) cation i.e. Pr^{3+}, and the surrounding ligand. These interactions lead to the contraction of 4f the wave function of metal ions, which establishes that the metal-ligand electronic repulsion and L-S interaction is responsible for the reduction in covalent characters.

In comparison to transition metal complexes, lanthanide complexes were found to have a lower value of bonding parameter ($b^{1/2}$), which confirms that the participation of 4f-orbitals in bonding is negligible. Ligand with a higher value of $b^{1/2}$ introduces more covalent characters in the M-L bond as compared to thiazole derivative ligands, which is confirmed by Nephelauxetic ratio (β), Sinha's covalency (δ%), and covalency parameter (η), i.e. angular overlap.

$$\beta = \upsilon_c/\upsilon_f \text{ ----------(15)}$$
$$b^{1/2} = [(1-\beta)/2]^{1/2} \text{ ---------- (16)}$$
$$\delta = [1-\beta/\beta\ ] \text{ X } 100 \text{----------(17)}$$
$$\eta = [1 - \beta^{1/2} / \beta^{1/2}] \text{ ----------(18)}$$
$$K' = P_{obs} /\upsilon T_6 \text{ ----------(19)}$$

Thermodynamic efficiency of Transition

$$(TET) = \frac{\text{Work Function}}{\text{Energy absorbed}}$$

By using thermodynamic relation-

$$A = E - TS, \text{ and } S = K \ln P_{obs}$$

The following relation is obtained-

$$A = E - KT \ln P_{obs} \text{---------- (20)}$$

Where,

A = Work function (cm^{-1})

E = Energy absorbed for hypersensitive transition (cm^{-1})

K = Boltzmann Constant = 0.6945 cm^{-1}

T = Absolute Temperature

P_{obs} = Oscillator strength of transition

S = Absolute energy

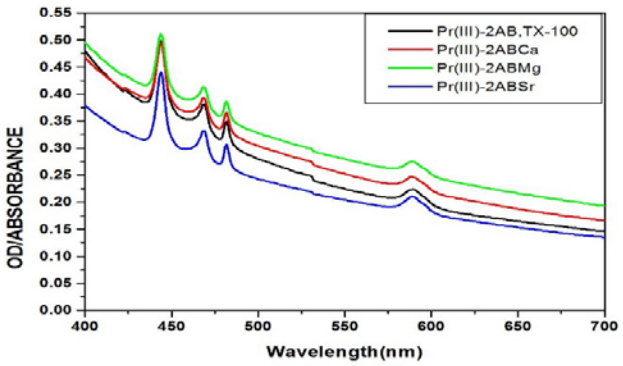

Fig. 1 A comparative UV-visible electronic absorption spectra of Pr(III)-2AB system with co-doping of Ca, Mg, Sr (II) ion in TX-100 (Micellar) Medium.

Results and Discussion

Orbital Interactions Parameters

The Slater Condon (F_K), Lande (ζ_{4f}) and Racah (E^k) are some of the most important interaction parameters. Among F_2, F_4, F_6, and ζ_{4f} parameters, F_2 and ζ_{4f} parameters decrease in comparison to free lanthanide (III) ions (Table-2). The result shows the expansion in 4f-orbitals during complex formation, which was expected to decrease the interelectronic repulsions and spin-orbit interaction. Variation in values of the "Racah Parameters" (E^k) or Energy parameters (E^1, E^2, and E^3) and Slater-Condon (F_K) parameters for different systems in the micellar medium.

E^1 - Pr(III)-2AB > Pr(III)-2AB-Mg^{2+} > Pr(III)-2AB-Sr^{2+}> Pr(III)-2AB-Ca^{2+}

E^2 - Pr(III)-2AB > Pr(III)-2AB-Mg^{2+}> Pr(III)-2AB-Sr^{2+}> Pr(III)-2AB-Ca^{2+}

E^3 - Pr(III)-2AB > Pr(III)-2AB-Mg^{2+}> Pr(III)-2AB-Sr^{2+} > Pr(III)2AB-Ca^{2+}

F_2 - Pr(III)-2AB > Pr(III)-2AB- Mg^{2+}> Pr(III)-2AB-Sr^{2+} > Pr(III)-2AB-Ca^{2+}

F_4 - Pr(III)-2AB-Mg^{2+} > Pr(III)-2AB-Ca^{2+} > Pr(III)-2AB > Pr(III)-2AB-Sr^{2+}

F_6 - Pr(III)-2AB-Mg^{2+} >Pr(III)-2AB > Pr(III)-2AB-Ca^{2+} > Pr(III)-2AB-Sr^{2+}

Variations in the value of Lande's parameter or Spin-Orbit Coupling (ζ_{4f}) Constant Parameter are as stated below-

ζ_{4f} -Pr-(III)-2AB > Pr(III)-2AB-Mg^{2+}> Pr(III)-2AB-Ca^{2+} > Pr(III)-2AB-Sr^{2+}

For Pr(III)-2AB in the micellar system, E_{cal} is 22599.5, and E_{exp} is 22598.87 for the $^3H_4 \rightarrow {}^3P_1$ transition. After co-doping of Ca^{2+}, $E_{cal.}$ remains same, but in case of Pr(III)-2AB-Mg^{2+} and Pr(III)-2AB-Sr^{2+} a slight decreased is observed in E_{exp} i.e. 22547.08. Deviation in R.M.S. ($\sigma_{\pm}$) is very small for all the systems, which varies from 0.53 to 0.64 (Table -1) RMS is in the typical error range of the Judd-Ofelt parameter fitting, which indicates good agreements between the experimental and calculated results.

Bonding Parameters

The value of β for Pr(III)-2AB in a micellar system, was found to be less than 1 for $^3H_4 \rightarrow {}^3P_1$ (0.998933), and while it was found to be more than 1 for $^3H_4 \rightarrow {}^3P_2$, $^3H_4 \rightarrow {}^3P_0$ and $^3H_4 \rightarrow {}^1D_2$ i.e. 1.00339, 1.001038, and 1.00085 respectively. The value of δ% was observed as negative for $^3H_4 \rightarrow {}^3P_2$, $^3H_4 \rightarrow {}^3P_0$, and $^3H_4 \rightarrow {}^1D_2$, i.e. -0.33784, -0.10373, and -0.08489 respectively. The value of covalence angular overlap varies from 0.000425 to 0.001691 (Table 3). For Pr(III)-2AB co-doped with Ca^{2+} in the micellar system value of β, δ%, and covalence angular overlap was found to be similar to the un-doped Pr(III)-2AB system for the above-mentioned transitions which suggest that the doping with Ca^{2+} doesn't make any influence on M-L bond nature (Table-4). The value of β for Pr(III)-2AB co-doped with Mg^{2+} in a micellar system, was found to be less than 1 i.e. 0.997868 for $^3H_4 \rightarrow {}^3P_1$, and $^3H_4 \rightarrow {}^1D_2$ while it was found to be more than 1 for $^3H_4 \rightarrow {}^3P_2$, and $^3H_4 \rightarrow {}^3P_0$ transitions i.e. 1.002257 and 1.001038 (Table-5) respectively, which suggests that the presence of more covalent

Compound		Pr(III)-2AB		Pr(III)-2AB-Ca^{2+}		Pr(III)-2AB-Mg^{2+}		Pr(III)-2AB-Sr^{2+}	
S.N.	Levels	E_{cal}	$E_{obs.}$	E_{cal}	$E_{obs.}$	E_{cal}	E_{exp}	E_{cal}	$E_{obs.}$
1	$^3P_2$	22599.5	22598.87	22599.51	22598.87	22574.08	22573.36	22548.5	22547.91
2	$^3P_1$	21344.85	21344.72	21367.64	21367.52	21322.13	21321.96	21367.62	21367.52
3	$^3P_0$	20767.59	20768.43	20767.61	20768.43	20767.38	20768.43	20767.57	20768.43
4	$^1D_2$	16992.39	16992.35	16992.39	16992.35	16949.25	16949.15	16992.45	16992.35
5	R.M.S. (σ)deviation (±)	0.60		0.53		0.64		0.60	

Table-1: $E_{Exp.}$ and $E_{Cal.}$ values of energy (in cm^{-1}) for different energy levels of Pr(III)-2AB system, and Co-doping of Ca^{2+}, Mg^{2+}, and Sr^{2+} metal ions in micellar (TX-100) medium

S.N.	Parameters	Pr(III)-2AB	Pr(III)-2AB-Ca^{2+}	Pr(III)-2AB-Mg^{2+}	Pr(III)-2AB-Sr^{2+}
1	E^1	4508.842	4502.651	4507.734	4505.26
2	E^2	23.5856	23.55322	23.5798	23.56686
3	E^3	455.8654	455.2395	455.7534	455.5033
4	F_2	307.1041	306.6825	307.0287	306.8602
5	F_4	76.1208	63.76157	80.88295	44.57286
6	F_6	6.783416	5.943737	7.083275	4.661073
7	ζ_{4f}	761.2991	755.2894	756.6863	729.1317
8	%r ζ_{4f}	-1.78509	-0.98159	-1.16836	2.515676
9	%r F_2	-2.57419	-2.43336	-2.54898	-2.4927
10	F_4/F_2	9.89073	9.89073	9.89073	9.89073
11	F_6/F_2	0.051738	0.051738	0.051738	0.051738
12	E^1/E^3	0.247866	0.207907	0.263438	0.145255
13	E^2/E^3	0.022088	0.019381	0.02307	0.01519

Table -2: The calculated value of the interaction parameters: (i) Slater-Condon F_k (cm^{-1}), (ii) Spin-Orbit interaction-Lande ζ_{4f} (cm^{-1}), (iii) Racah E^k (cm^{-1}) parameters (iv) Hydrogenic Ratio (F_4/F_2), (F_6/F_2), (v)(E^1/E^3), and (E^2/E^3) for Pr(III)-2AB system and Co-doping of Ca^{2+}, Mg^{2+}, and Sr^{2+} metal ions in micellar medium

S.N..	Transition	λc(nm)	Vc (cm^{-1})	(β)	($b^{1/2}$)	δ%	(η)
1	$^3H_4 \rightarrow {}^3P_2$	442.5	22598.87	1.00339	0.041169	-0.33784	0.001691
2	$^3H_4 \rightarrow {}^3P_1$	468.5	21344.72	0.998933	0.0231	0.106838	0.000534
3	$^3H_4 \rightarrow {}^3P_0$	481.5	20768.43	1.001038	0.022786	-0.10373	0.000519
4	$^3H_4 \rightarrow {}^1D_2$	588.5	16992.35	1.00085	0.020611	-0.08489	0.000425

Table-3: The computed values of bonding parameters: (i) Nephelauxetic ratio (β), (ii) Bonding ($b^{1/2}$), (iii) Sinha Covalency (δ %) (iv) Covalency-Angular Overlap (η) parameters of Pr(III)-2AB system in micellar (TX-100) medium

S.N.	Transition	λc(nm)	Vc (cm^{-1})	(β)	($b^{1/2}$)	δ%	(η)
1	$^3H_4 \rightarrow {}^3P_2$	442.5	22598.87	1.00339	0.041169	-0.33784	0.001691
2	$^3H_4 \rightarrow {}^3P_1$	468	21367.52	1.00	0	0	0.000000
3	$^3H_4 \rightarrow {}^3P_0$	481.5	20768.43	1.001038	0.022786	-0.10373	0.000519
4	$^3H_4 \rightarrow {}^1D_2$	588.5	16992.35	1.00085	0.020611	-0.08489	0.000425

Table 4: The Calculated values of bonding parameters: (i) Nephelauxetic ratio (β), (ii) Bonding ($b^{1/2}$), (iii) Sinha Covalency (δ %) (iv) Covalency-Angular Overlap (η) Parameters of Pr(III)-2AB Co-doped with Ca^{2+} metal ion in micellar (TX-100) medium

S.N.	Transition	Λc (nm)	Vc (cm^{-1})	(β)	($b^{1/2}$)	δ%	(η)
1	$^3H_4 \rightarrow {}^3P_2$	443	22573.36	1.002257	0.033596	-0.22523	0.001127
2	$^3H_4 \rightarrow {}^3P_1$	469	21321.96	0.997868	0.032651	0.213675	0.001068
3	$^3H_4 \rightarrow {}^3P_0$	481.5	20768.43	1.001038	0.022786	-0.10373	0.000519
4	$^3H_4 \rightarrow {}^1D_2$	590	16949.15	0.998305	0.029111	0.169779	0.000849

Table 5: The calculated values of various bonding parameters: (i) Nephelauxetic ratio (β), (ii) Bonding ($b^{1/2}$) (iii) Sinha Covalency (δ %) (iv) Covalency-Angular Overlap (η) parameters of Pr(III)-2AB Co-doped with Mg^{2+}metal ion in micellar (TX-100) medium

S.N.	Transition	λc(nm)	Vc (cm^{-1})	(β)	($b^{1/2}$)	δ%	(η)
1	$^3H_4 \rightarrow {}^3P_2$	443.5	22547.91	1.001127	0.023742	-0.11261	0.000563
2	$^3H_4 \rightarrow {}^3P_1$	468	21367.52	1.00	0	0	0.000000
3	$^3H_4 \rightarrow {}^3P_0$	481.5	20768.43	1.001038	0.022786	-0.10373	0.000519
4	$^3H_4 \rightarrow {}^1D_2$	588.5	16992.35	1.00085	0.020611	-0.08489	0.000425

Table 6: The calculated values of bonding parameters: (i) Nephelauxetic ratio (β), (ii) Bonding ($b^{1/2}$), (iii) Sinha Covalency (δ %) (iv) Covalency-Angular Overlap (η) parameters of Pr(III)-2AB Co-doping of Sr^{2+} metal ion in micellar (TX-100) medium.

nature in M-L bond. The value of δ% for $^3H_4 \rightarrow {}^3P_2$, $^3H_4 \rightarrow {}^3P_0$ was observed negative i.e. -0.22523, -0.1.373. The covalence angular overlap value ranges from 0.000849 to 0.001127 (Table -5).

Conclusion

For Pr(III)-2AB micellar system co-doped with Sr^{2+}, the β value was obtained equal to 1.00 for $3H_4 \rightarrow {}^3P_1$ and more than 1 for $^3H_4 \rightarrow {}^3P_2$, $^3H_4 \rightarrow {}^3P_0$, and $^3H_4 \rightarrow {}^1D_2$ i.e. 1.001127, 1.001038, and 1.0085 respectively. The value of δ% for $^3H_4 \rightarrow {}^3P_2$, $^3H_4 \rightarrow {}^3P_0$, and $^3H_4 \rightarrow {}^1D_2$ was found to be negative i.e. -0.11261, -0.10373, and -0.08489. The covalence angular overlap value varies from 0.0 to 0.00563 (Table -6). In the Pr(III)-2AB, co-doped with Ca^{2+}, Mg^{2+}, and Sr^{2+} system, the value of the bonding parameter ($b^{1/2}$) in positive indicates a more percentage of covalency in the metal-ligand bond. In contrast, the -ve value reflects the ionic nature in the metal-ligand bond. Smaller value (<1) of bonding parameters (β, δ, and η) corresponds to fewer covalent characters, while higher (>1) values of bonding parameters (β, δ, and η) reveals strong covalent characters in metal-ligand bond. The decrease in the value of F_k and E_k parameters indicates the reduction in inter-electronic repulsion and spin-orbit interactions, which suggests an expansion of the orbital of the central metal ion on complexation, following the theory of f→f transition reported earlier.

Conflict of Interest Statement

Authors do not have any conflict of interest.

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