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INTENSITY PARAMETERS OF Sm(III) COMPLEXES WITH AMIDE GROUP CONTAINING LIGANDS: A COMPARATIVE STUDY

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Abstract: A comparative study of intensity parameters of doped systems of Sm(III) complexes have been done. Three aminopyridine derivatives as ligands have been taken for investigations with Samarium trivalent metal ion in alcoholic and micellar medium (Triton X-100). The Electronic spectra were recorded in ultraviolet-visible range. The intensity parameters calculated are oscillator strength and Judd-Ofelt parameters.

Keywords: A comparative study, Alcoholic, Micellar Medium, Ultraviolet-Visible Range.

I. INTRODUCTION

Samarium, like other rare earths, is becoming increasingly valuable in a world where reliance on high-tech is increasing. Rare earth metals are becoming increasingly important in the production of high-tech electronic devices. Samarium has numerous applications. It is used in the production of alloys, optical glass, carbon-arc lamps, lasers, and optical masers. The element samarium is used in sensitizers and nuclear reactors. Samarium can also be used as a catalyst in many reactions and has medical applications. [1-3]

The spectral intensities of the bands of Sm^{+3} ion in a $SeOCl_2 + SnCl_4$ laser liquid were observed by Y.C. Ratnakaram and S. Buddhudu. The Judd Ofelt parameter was evaluated using a least square fit method, and the spectral intensities measured from the profile of the bands of the ion studied are strongly correlated with the theoretical intensities, establishing the validity of the Judd Ofelt theory [4]. S.A.Kalyani et al. investigated lanthanide (III) complexes of N-arylthioureas. They had analysed the electronic spectra and calculated the spectral parameters. The molar conductance values revealed that a few complexes were electrolytic in nature while others were not [5].

II. EXPERIMENTATION

Samarium chloride and carbonate (Indian Rare Earths Limited, India) of 99.9% purity were used. Stock solution of Sm (III) was prepared by dissolving appropriate amount of Samarium chloride or Samarium carbonate in double distilled water. Triton–X-100 was used to provide micellar medium. Triton-X-100 (1.8 x 10-2 M, 100 CMC) is a non-ionic surfactant. Three amino derivatives taken as ligands are as follows: -

1. N-(2′-pyridyl)-4-hydroxybenzamide (N2P4HB)
2. N-(2′-pyridyl)-3,5-dinitrobenzamide (N2P3,5DB)
3. N-(2′-pyridyl)-4-carboxamide but-1-oic acid (N2P4C1BA)

EC Double beam UV-VIS Spectrophotometer with quartz cell of 10 mm light path was used for electronic spectral measurement at Green Chemistry Research Centre, P.G. Dept. of Chemistry, Govt. Dungar college (NAAC A-Grade) Bikaner, (Raj.)

The absorption spectra of each system were recorded in various medium i.e. in alcoholic medium and in micellar medium intensity parameters include oscillator strengths and Judd-Ofelt intensity (T_λ) parameters. Calculation of parameters done as given in literature [6].

The oscillator strength(P) values for Sm(III) complexes are of the order of 10^{-6}, indicating that the transitions are forbidden. The ligand has a large influence on the intensity of the hypersensitive transition in Sm(III) complexes. Higher oscillator strength (P) values indicate less symmetry in complexes [7].

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The higher P and parameter values of salt solutions in comparison to metal aqueous show the involvement of a metal ion's 4f-orbital. These parameters also show higher values with more soluble salts [8-10]. The negative value of the T_2 parameter is meaningless. This could be due to the appearance of the f-d transition in the visible region, or it could be compensation for the excessively large oscillator strength computed for T_4 and T_6 parameters [11].

Table - 1
Computed values of oscillator strength ($P \times 10^6$) for Sm(III) complexes of aminopyridine derivatives in alcoholic and micellar medium

S.No.	LEVEL	$^4I_{13/2}$		$^4I_{11/2}$		$^4F_{3/2}$		$^4G_{5/2}$		r.m.s. dev(±)
	COMPOUND	P_{exp}	P_{cal}	P_{exp}	P_{cal}	P_{exp}	P_{cal}	P_{exp}	P_{cal}	
1	N2P4HB(Alcoholic)	4.42	-2.85	4.89	-1.62	7.16	1.19	5.68	1.36	6.65
2	N2P4HB(Micellar)	5.05	-3.65	6.93	-9.12	8.34	2.88	6.36	-3.11	7.92
3	N2P3,5DB(Alcoholic)	5.14	-4.75	8.66	-2.93	9.28	4.83	6.90	-7.76	8.97
4	N2P3,5DB(Micellar)	5.01	11.09	8.36	5.00	9.11	-6.80	7.03	-3.85	7.05
5	N2P4C1BA(Alcoholic)	1.90	1.90	2.08	2.08	-1.16	-1.17	-5.09	-5.10	7.01
6	N2P4C1BA(Micellar)	-3.27	-3.27	1.58	1.58	6.51	6.52	-1.26	-1.26	7.59

Table - 2
Computed values of T_λ and T_4 / T_6 parameters for Sm(III) complexes of aminopyridne derivatives in alcoholic and micellar medium

S.N.	COMPOUND	$T_2 x10^{10}$	$T_4 x10^{10}$	$T_6 x10^{10}$	T_4/T_6
1	N2T4HB (Alcoholic)	21.32	102	-72	-1.416
2	N2T4HB (Micellar)	50.69	-261	-40.2	6.488
3	N2T3,5DB (Alcoholic)	86.4	-638	-13.0	49.13
4	N2T3,5DB (Micellar)	-1217	43.14	221	0.1952
5	N2T4C1BA (Alcoholic)	-2.10	-402.83	91.8	-4.388
6	N2T4C1BA (Micellar)	117.0	-1037.7	69.7	-14.88

Table - 3
Maximum and Minimum spectral parameters for Sm (III) complexes of aminopyridine derivatives in alcoholic medium

S.No.	Spectral Parameters	Maximum		Minimum	
		Ligand	Value	Ligand	Value
1	T_2	N2P3,5DB	86.4×10^{-10}	N2P4C1BA	-2.1×10^{-10}
2	T_4	N2P4HB	102.0×10^{-10}	N2P3,5DB	-638.0×10^{-10}
3	T_6	N2P4C1BA	91.8×10^{-10}	N2P4HB	-72.0×10^{-10}
4	T_4 / T_6	N2P3,5DB	49.138	N2P4C1BA	-4.388

Table -4
Maximum and Minimum spectral parameters for
Sm (III) complexes of aminopyridine systems in micellar medium

S.No.	Spectral Parameters	Maximum		Minimum	
		Ligand	Value	Ligand	Value
1	T_2	N2P4C1BA	117.0×10^{-10}	N2P3,5DB	-1217×10^{-10}
2	T_4	N2P3,5DB	43.1×10^{-10}	N2P4C1BA	-1037×10^{-10}
3	T_6	N2P3,5DB	221.0×10^{-10}	N2P4HB	-40.24×10^{-10}
4	T_4 / T_6	N2P4HB	6.488	N2P4C1BA	-14.88

III. RESULTS AND DISCUSSION

Present study on Sm (III) systems with saturated alcoholic and micellar solutions of three aminopyridine derivatives is based on doped crystal phenomenon. Intensity parameters have been described in a saturated solution of three aminopyridine derivatives. The intensity parameters are Oscillator Strength (P) and Judd- Ofelt parameters ($T\lambda$). Use of computational chemistry has been explored in order to develop better and easier methods of calculations The equations described in the literature were used to calculate the various intensity parameters. In the case of Sm3+, four bands have been observed and recorded in the 400-900 nm range. In computing oscillator strength values, the value half band width was determined by resolving the observed bands into a Gaussian shape curve, which allowed for better investigations of different parameters.

Table 1 shows the intensity parameters for Sm (III) aminopyridine derivative complexes, while table 2 shows the Judd-Ofelt parameters. Table 3 and table 4 show the minimum and maximum value of parametrs calculated in alcoholic and micellar medium. The value for oscillator strength is found to be greater in alcoholic medium than in micellar medium. In alcoholic medium, Samarium complex with N2P3,5DB had the highest oscillator strength of 9.28, while in micellar medium, Samarium complex with N2P3,5DB has the highest oscillator strength of 9.11.

IV. CONCLUSION

The current comparative study describes six doped Sm (III) systems in alcohol and micellar medium. Each system's solution spectra were recorded in the UV-Visible range. The spectral parameters of these doped systems were evaluated using their spectral data. Calculations were performed using the partial and multiple regression methods.

On the basis of computed data comparative investigations of Oscillator strength have been described with respect to ligands and medium.

For Sm (III)-aminopyridine systems in alcoholic medium
N2P3,5DB > N2P4HB> N2P4C1BA

For Sm (III)-aminopyridine systems in micellar medium
N2P3,5DB > N2P4HB > N2P4C1BA

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