ESTIMATION OF REGRESSION MODEL FOR THE SUSCEPTIBLE TRANSITIONS OF COMPLEX SYSTEMS

[1]Anil Dhankhar, [2]Akshya Raj Choudhary
[1, 2] Asstt. Professor
[1, 2] Department of MCA,
[1,2]Rajasthan Institute of Engineering & Technology, Jaipur, India

Abstract - The significance of computational models for the development of material science is one of the important emerging technological fields where, absorption spectra of lanthanide ions have been a subject of several investigations because of their possible use as laser materials, diagnostic tools and sensors. Study of absorption spectra in visible and near infrared regions yields useful information regarding energy and intensity parameters, and nature and probabilities of transitions. Statistical models, particularly regression models are extremely useful devices for extracting and understanding the essential features of a set of data. These models however are nearly always approximate description of more complicated processes, and because of this inexactness, the study of the variation in the results of analysis with minor modifications of the way the problem is formulated becomes important. It is important to develop easy models of computation and communication which has significant of potential applications of their complexes in many important areas of biology and medicines.
The present investigation deals with the development of a regression model based on C language and its applicability for the determination of spectral, energy & intensity parameters of lanthanide complexes in different medium. Various energy and intensity parameters such as Racah (E^K), Slater-Condon (F_K), Lande' (ζ_{4f}), Oscillator strength (P) and Judd-Ofelt parameter ($T\lambda$) etc. have been computed using partial and multiple regression methods.

Key word: - Regression model, lanthanides, spectra

INTRODUCTION

The Statistical models, particularly regression models are extremely useful devices for extracting and understanding the essential features of a set of data. These models however are nearly always approximate description of more complicated processes, and because of this inexactness the study of the variation in the results of as analysis with minor modifications of the way the problem is formulated becomes important. Chemical physics provides fundamental tool to develop lanthanide chemistry, which has been increasingly significant in the last few years due to the wide variety of potential applications of their complexes in many important areas of biology and medicines. The absorption spectra of lanthanide ions have been a subject of several investigations because of their possible use as laser materials, diagnostic tools and sensors. Study of absorption spectra in visible and near infrared regions yields useful information regarding energy and intensity parameters, and nature and probabilities of transitions. The present investigation deals with the development of a novel computational regression model and its applicability for the determination of spectral, energy & intensity parameters of semicarbazone complexes with Sm(III) in different medium. Various energy and intensity parameters such as Racah (E^K), Slater-Condon (F_K), Lande' (ζ_{4f}), Oscillator strength (P), Judd-Ofelt parameter ($T\lambda$) have been computed and nephelauxetic ratio (β) and Bonding parameter ($b^{1/2}$) have been evaluated. Model has been compared with the existing methods and it is found that developed model is not only easier to use but provide better sensitivity in results and also significant in micellar medium. Lanthanide chemistry has been increasingly significant in the last few years due to the wide variety of potential applications of their complexes in important areas of biology and medicines [1-4].

EXPERIMENTAL

The Semicarbazones were synthesized by refluxing semicarbazide- in equimolar ratio with cinnamaldehyde, 4-aminophenazone, p-anisaldehyde, 3-chlorobenzaldehyde and 2-chlorobenzaldehyde for 5 to 6th at temperature 70 to 80°C as per reported procedure. The compounds were purified and crystallized in ethanol. The saturated solution of cinnamaldehyde semicarbazone (CSC), 4-aminophenazone semicarbazone *(p-APSC)*, p-anisaldehyde semicarbazone (p-ASC), 3-chlorobenzaldehyde semicarbazone (3-CBSE) and 2-chlorobenzaldehyde semicarbazone (2-CBSE) were prepared in suitable solvent and lanthanide salt were added to the solution. Triton-X-100 surfactant was used ($1.8 \times lO^{-2}$ M, 100 CMC). The solution spectra of the system were recorded by using standard spectrophotometer in the visible region [5].

The calculation for various Electronic parameters was made by computerized statistical method reported earlier and the program developed by using C language. Results were compared with existing program and technique.

RESULTS AND DISCUSSION

The various energy parameters include Oscillator strength *(P)*, Slater-Condon parameters *(F_2' F_4* and *F_6)*, nephelauxetic ratio (β), bonding parameter *($b^{1/2}$)*, Racah parameter *(E^1, E^2* and E^3), Lande parameter *(ζ_{4f})'* percentage reduction in F_2 parameter (% *rF_2)'* and percentage reduction in ζ_{4f} parameter (% *$r\zeta$)* have been reported in Tables (1, 2). Wong method has been used to calculate the Slater-Condon parameter *(FK)* and Lande's parameter *(ζ_{4f}).* In the complexes of Nd (III) the decrease in interelectronic repulsion and spin orbit interactions which suggest expansion of the central metal ion orbital on complexation and is in accordance with the theory of *f* ↔ *f* transition reported earlier [6-8]. The values of Slater~Condon parameter *(F_K)* were found to decrease in comparison to free metal ion. The values of Lande's parameter *(ζ~f)* were also found to be decreasing.

The decrease in computed values of spin orbit interaction parameter (ζ_{4f}) and Slater-Condon parameter *(F_K)* in comparison to free ion values show clearly symmetry change around the metal ion in the solution. The small deviations for the calculated and observed values suggest the validity of Judd-felt [9] equations for f ↔ f transition for the present study. The parametric values provide useful information regarding the coordination behaviour of Nd (III) ion. On comparing the results for both mediums Oscillator strength *(P),* Slater-Condon parameters *(F K)'* Racah parameter *(EK)* and nephelauxetic ratio have been found to be increasing in micellar medium. The decreasing value of Lande's parameter *(s.v)* in micellar medium has been observed. Lesser value of Slater-Condon parameter than free ion value suggests the decrease in spin orbit interaction and interelectronic repulsion indicating a general red shift, but less decrease in value of *F K* has been observed for micellar medium. Greater values of Racah parameter *(E_K)* has been observed. Also the value of β has been found to be less than one of micellar medium.

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Table 1. Computed Values of Oscillator Strength of the Brands Observed for Nd (III) Ion doped in Saturated Solution of Semicarbazones

Level	CSC+Nd 6 PexpxlO6 PcalxlO		CSC+Nd (Micellar) PexpxlO. PcalxlO6		p-ASC+Nd PexpxlO. PcalxlO6		p-ASC+Nd (Micellar) PexpxlO. PcalxlO6		2-CBSE+Nd PexpxlO. Pcalxlo"		2-CBSC+Nd (Micellar) Pexpxlo" PcalxlO6		p.APSC+Nd PexpxlO6 PcalxlO6		p-APSC+Nd (Micellar) PexpxlO' PcalxlO'		3.CBSC+Nd PexpxlO6 PcalxlO'		3-CBSC+Nd (Micellar) PexpxlO6 PcalxlO6	
2 PV 2	3.420	0.716	4.39	0.908	1.19	0.996	2.380	0.780	1.36	.555	2.75	0.659	1.41	1.20	2.21	1.380	1.67	0.771	2.23	1.340
4 G1	3.900	0.230	1.11	0.187	2.71	0.212	1.440	0.194	2.05	0.133	1.74	0.187	0.472	0.347	2.21	0.278	1.3	0.260	2.21	0.229
4 G9; 2	4.68	1.750	1.46	1.710	2.46	1.960	2.670	1.640	2.41	1.170	1.62	1.520	4.83	2.82	2.46	2.590	2.09	1.990	2.47	2.650
2 *G91 2*	1.560	.445	2.72	0.405	2.10	0.459	1.170	0.400	1.85	0.283	2.52	0.375	1.38	.697	3.01	0.608	3.60	0.506	2.80	0.634
4 *G7h*	3.500	3.570	3.58	3.960	5.49	4.570	2.440	3.550	2.91	2.880	3.5	3.340	7.82	6.54	5.69	6.090	2.63	4.350	5.18	6.050
4 *GSh*	9.360	10.500	13.50	14.200	16.60	18.200	9.850	11.100	13.20	13.600	11.80	12.700	26.4	26.4	21.00	23.100	16.30	17.900	19.90	22.100
4 F9; 2	.543	.559	3.19	0.374	1.15	0.438	0.263	0.436	2.35	0.295	1.64	0.441	1.27	.826	1.41	0.556	1.01	0.650	1.76	0.630
4 *F7h*	4.810	4.880	2.90	2.830	2.66	3.260	3.260	3.570	2.87	2.350	4.12	3.720	6.28	6.91	3.37	4.140	5.95	6.690	3.89	4.930
4 *FSh*	4.300	6.230	3.42	4.970	2.68	5.650	3.380	5.260	2.03	3.580	3.06	5.050	5.35	9.36	4.55	7.370	4.12	7.070	5.28	7.950
4 *F3h*	1. 820	2.630	3.10	2.960	1.82	3.260	2.120	2.670	2.21	1.880	2.36	2.330	2.14	4.26	3.25	4.470	2.97	2.880	3.05	4.440

Table.2 Computed values of Energy (Fk, 4f, Ek, % r 4r, and b1/2) Nd(lII) Ion Doped in Saturated Solution of Various Semicarbazones of Carboxyl Compounds

Compound	*F2*	*F4*	*F6*	*%rF2*	*(,41*	*%r*	*El*	*E2*	*E3*	13	*b1/].*
CSC+Nd	328.83	51.79	5.27	0.7041	849.54	3.90	5059.98	23.38	491.64	0.9917	0.064
CSC+Nd (in Micellar Medium)	328.9	52.42	5.29	0.6816	832.88	5.78	5081.93	23.19	492.30	0.9919	0.063
P – ASC+ND	329.57	51.88	5.31	0.4769	843.68	4.56	5076.58	23.45	491.97	0.9940	0.055
P-ASC +Nd (in Micellar Medium)	329.59	52.24	5.30	0.4741	835.07	5.53	5083.88	23.33	492.93	0.9940	0.055
2-CBSC +Nd	329.99	51.87	5.31	0.3505	832.66	5.81	5078.99	23.51	492.70	0.99530	0.049
2- CBSC+ND (in Micellar Medium)	328.57	52.33	5.29	0.7828	843.63	4.57	5077.48	23.19	491.53	0.9909	0.067
P - APSC+Nd	327.96	51.38	5.29	0.9637	860.28	2.68	5046.89	23.42	488.88	0.9891	0.073
P-APSC+Nd (in Micellar Medium)	329.26	52.10	5.35	0.5917	841.54	4.8	5087.78	23.27	490.77	0.9930	0.059
3-CBSC +ND	328.86	52.31	5.31	0.6917	839.64	5.02	5080.99	23.23	491.74	0.9919	0.064
3 –CBSC +Nd (in Micellar Medium)	329.08	52.11	5.34	0.6263	843.66	4.56	5085.42	23.35	490.62	0.9925	0.061