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The Evaluation of F-F Spectra of Some ER (Iii) Ternary Complexes Containing Crown Ethers and Amino Acids & Computation of Spectral Parameters Using the Spectra

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Abstract: ***The f-f electronic transition spectra of ternary complexes of Er(III) metal ion [M] prepared by taking crown ethers [L_1]:18–Crown–6, benzo-18-Crown-6 & dibenzo-18-Crown-6 & the amino acids [L_2]: glycine, β-alanine & L-arginine, respectively, in various metal- ligands stoichiometries [M:L_1:L_2] ratio, have been recorded in visible region, in solution. The intensity of the ten selected bands of the f-f electronic transition spectra of these complexes have been analyzed & evaluated to explain nature of bonding, symmetry photophysical properties etc. The spectra have been quantified in terms ofenergy interaction parameters: such as Racah (E^k), Slator- Condon (F_k), Landé (ζ_{4f}), electric dipole intensity parameters in terms of Judd-Ofelt (T_2, T_4& T_6) & Oscillator strength (P_{osc}) and the bonding parameters: Nephelauxetic ratio (β) & co-valency ($b^{1/2}$).The JO analysiso fintensity parameters reveals that the value of T_2 determine the photophysical property, higher the value of T_2 ,higher the photoluminescence and the other JO parameters are associated with symmetry and structure. All these parameters have been computed using various statistical methods given by Wong &others. The variation in these parameters for the complexes with respect to the free ion shows the complexation reaction, change in symmetry around metal ion, structure of the complexes/ligand, nature of metal-ligand bond etc. The metal-ligands stoichiometric [Er:CW:AA] ratio of these complexes was found to be [1:3:2], in general& were determined by the Mole Ratio method.***

Keywords:*Er(III) ternary complexes, metal-ion, amino acids, crown ethers, f-f electronic spectra, energy, intensity and bonding parameters,*

I. INTRODUCTION

Recently in last two decades, there has been considerable interest in coordination chemistry of lanthanides, also called rare-earth elements, in solution, because the lanthanide complexes, specially ternary complexes, play important role in various biological systems to photonic devices[1-3]. This is especially due to the compatible size of lanthanide ions with the calcium ion and ability to bind tightly with it & ease with calcium ion is replaced. Smart & careful strategies need to be adopted for the search of new organic ligands which can enhance the photo luminescent properties through complication [4]. The lanthanide ternary complexes are, usually, prepared with, mainly with neutral crown ether molecule as primary ligand which forms stable core of the complex having oxygen – metal bonding. The Lanthanide - crown ether combination is quite stable as lanthanide ion gets fixed in size fitted crown ether cavity. The crown ether also act as sensitizer or antenna which absorb energy and transfer to the lanthanide ion for the efficient excitation & to enhance its photo luminescent property. Amino acids are taken as secondary ligand which removes the remaining water molecule in the coordination sphere to avoid radiation less deactivation [5-7]. The ternary complexes of type [Ln: CW: AA] are being used for photonic devices (OLED, LCD etc.) to magneto-luminescent applications (EDFA, MRI etc.)to biological fluorescent probe(LLBs).The such ternary complexes are also suitable the cleavage of phosphodiester bond, studying toxicity of metal ions & metal-detoxification etc.

In this communication we report the preparation of such ten ternary complexes of Er (III) by taking crown ethers: 18-crown-6, benzo-18-crown-6 & dibenzo-18-crown-6 and amino acids: glycine, β-alanine & arginine, in solution. The *f-f* transition spectra have been recorded in solution. The spectra have been evaluated & analyzed and spectral parameters, energy interaction parameters: such as Racah (E^k), Slator- Condon (F_k), Landé (ζ_{4f}), electric dipole intensity parameters in terms of Judd-Ofelt (T_2, T_4& T_6) &Oscillator

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strength (P_{osc}) and the bonding parameters: Nephelauxetic ratio (β) & co-valency ($b^{1/2}$)have been computed to explain the symmetry, ligand environment around the Er (III) ion, nature of Er (III)- ligand bonding using these spectra[8]

II. EXPERIMENTAL

A. Materials

All reagents, Er (III) acetate (Otto Chemika), crown ethers (Aldrich), amino acids (Himedia Lab, Biochemika) were of the highest purity (AR grade). The solvents Methyl cyanide (Qualikem) and methyl alcohol (Uvasol:Sigma-Aldrich) were of spectroscopic grade.

B. Method to record spectra

The stock solutions (0.01M) of the ligands: Crown ethers [L_1] namely, 18–Crown–6 [CE], Benzo 18–Crown–6 [CB] and dibenzo 18– Crown–6 [CD] and amino acids [L_2], namely, β-Alanine [AL], glycine [GY], and L-Arginine [AR] were prepared by dissolving the calculated mass of each of them in a minimum quantity of the mixture of CH_3OH and CH_3CN (whenever necessary) or in distilled water. The metal ion solution (0.01M) was prepared by dissolving the salt of Er (III) in double distilled water and was standardized by the conventional complex metric method.The sample solutions were prepared by taking the metal ion solution [M] and the ligand solutions [L_1]& [L_2] in stoichiometric ratio [M:L_1:L_2] of [1:3:1], [1:3:2], [1:1:3] and [1:2:3] to record the spectra. The electronic absorption spectra have been recorded by the measuring the absorbance (A) at different wavelengths, for each sample solution having 1:3:1, 1:3:2, 1:2:3 or 1:1:3 [M:L_1:L_2] metal-ligand stoichiometry at room temperature. The absorbance (A) of sample solution having 1:3:2 metal-ligand ratio is maximum and this indicate the metal-ligand stoichiometry. This also shows that there is maximum stacking of ligands around the metal ion thereby indicating the interaction between metal-ion and ligands.

III. RESULTS AND DISCUSSION

The intra *f –f* transitions 4*f* in orbitals of the lanthanides areresponsible for the *f –f* transitions spectra. These transitions are spin and parity or Lapporte forbidden transitions of low intensity. The Judd-Ofelt theory has been applied to interpret the low intensities of the transitions. Theshifting of transition peak toward the longer wavelength in the ligand environment as compared to free ion indicates the interaction of the stereo-environment around the central metal ion. This provide a lot of information about the various interactions such as interelectronic, spin –spin, spin-orbit and mixing of metal-ligand orbitals, nature of bonding etc. The ten bands corresponding to $^4F_{9/2}$, $^4S_{3/2}$, $^2H_{11/2}$, $^4F_{7/2}$, $^4F_{5/2}$, $^4F_{3/2}$, $^2H_{9/2}$, $^{\mathbf{4}}\mathbf{G_{11/2}}$, $^4G_{9/2}$&$^2G_{7/2}$ respectively, arising, from the ground state $^4I_{15/2,}$ transitions were identified. The absorbance & the intensity is maximum for hypersensitive transition ($^4I_{15/2}\rightarrow{}^4G_{11/2}$) and the shifting in peak is linked to co-valency of metal –ligand bond. The changes in values of all the parameters as compared to the free ion and also in the various metal and ligand [M:L_1:L_2] ratios i.e.[1:3:1, 1:3:2, 1:1:3, 1:2:3] is not much significant. Further, this shows that ligands have little effect on the spectral pattern. The absorption spectra have been analyzed to derive various spectral parameters. The values of energies (E) for peaks of various *f-f* transition bands, intensity & bonding, parameters of all the metal-ligand complexes are summarized in Table-1 & 2.

A. Energy Parameters

The energy level structure of $4f^N$ configurations arise as a result of columbic and spin-orbit interactions, which are expressed as inter electronic repulsion parameters, namely, Slator-Condon (F_k), Racah (E^k) and Landé parameters (ζ_{4f}), respectively: These parameter can be evaluated by solving Taylor series expansion equations [12]

$$Ej\left(F_k\zeta_{4f}\right)=E_{oj}\left(F_k^0,\zeta_{4f}^0\right)+\sum_{k=2,4,6}\frac{\partial E_j}{\partial F_k}\Delta F_k+\frac{\partial E_j}{\partial F_{4f}}\Delta\zeta_{4f}$$

Where E_{0j}= the zero order energy of level j.

$$F_k = F_k^0 + \Delta F_k$$
$$\zeta_{4f} = \zeta_{4f}^0 + \Delta\zeta_{4f}$$
$$\Delta F_k << F_k^0, \Delta\zeta_{4f} << \Delta\zeta_{4f}^0$$

The difference between the observed E_j values and zero-order ones, ΔE_j, can be expressed as:

$$\Delta E_j = \sum_{k=2,4,6}\frac{\partial E_j}{\partial F_k}\Delta F_k+\frac{\partial E_j}{\partial\zeta_{4f}}\Delta\zeta_{4f}$$

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The experimental energy of the observed level of lanthanide Er (III) ion are presented Table-1.These values are very small which indicate that a full matrix digonalization procedure leads to a good fit between observed and calculated energies. The magnitude of parameters F_2, F_4, F_6 and ζ_{4f} were computed using regression analysis and refined by the least squares techniques.
There is red shift and the slight decrease in the values of Slator-Condon (F_k), Racah (E_k) and Landé Parameters (ζ_{4f}) with respect to the free ion means mixing of metal & ligands orbitals indicating co-valency of Er-O bond. On complexation, contraction or expansion of wave function occurs, which is reflected by changes in values of $F_k$and ζ_{4f} parameters with respect to the corresponding free ion values. For all the complexes of the metal ion the order of Slator-Condon parameter is found to be $F_2>F_4>F_6$ with the each ligand system . The values of Racah (E_k), Slator-Condon (F_k) and Landé Parameters (ζ_{4f}) are summarized in Table-2.
The decreases in the values of the Landé parameter (ζ_{4f}) is more than Slator-Condon (F_k) parameter indicating that the ligands affect the spin oprbit coupling more than the electrostatic repulsion.

B. Intensity Parameters

The spectrophotometric method is very convenient for the determination of the Judd-Of let (T_λ) intensity parameters. The low intensity of transitions is expressed in terms of oscillator strength (P_{obs}) and this was explained by Judd-Oflet theory.

1) Oscillator Strength: The low intensity of bands of Lapporte forbidden *f –f* transitions have been explained by Judd-Ofelt.The observed intensity is due to the contributions of induced electric dipole (P_{ed}), and other contributions of magnetic dipole (P_{md}) & electric quadruple (P_{eq}) are very small. This is measured in terms of oscillator strength (P_{osc}). The theoretical oscillator strength (P_{cal}) of electric dipole transition (between states SLJ & S'L'J') with f^N configuration can be calculated using equation (1)-.

$$P_{cal} = \frac{8\pi^2 m c \sigma}{3h(2J+1)} \chi \sum_{\lambda=2,4,6} T_\lambda |\langle SLJ \| U^\lambda \| S'L'J' \rangle|^2 \quad (1)$$

Where m is electron mass, c is speed of light, h is Plank constant, χ is field correction factor $\chi = (n^2+2)^2/9n$, where n is the refractive index, σ transitive wave number & 2J + 1, the degeneracy of |SLJ>& $\| U^\lambda \|^2$ represent the square of the reduced matrix element of the tensor operator U^λ connecting initial and final state[9-11]. The experimental oscillator strength of each band the *f-f* transition has been computed using the following equation(2)

$$P_{exp} = 4.138 \times 10^{-9} \int \epsilon_{max} (\nu_{1/2}).\Delta \nu_{1/2} \quad (2)$$

Where $\nu^{1/2}$= half band width and ε_{max} = molar extinction coefficient.
The values are summarized in the Table-1 for all the metal-complexes.

2) RMS Deviation (σ_{rms}): The σ_{rms} values [12-13] for Er(III) metal-complexes range from 103.36×10^{-6} to 113.17×10^{-6} for different metal-ligand stoichiometry, respectively. The σ_{rms} values have been summarized in Table-1. The small values of σ_{rms}deviations indicate the suitability of the relations used.

3) Judd-Ofelt Parameters-These Judd-Ofelt (T_λ,λ=2,4&6) parameters are indicative of stereo environment around the metal ionThe trend of Judd-Ofelt parameters have been found in Er (III) complexes is $T_2<T_4<T_6$. The values of T_4/T_6 ratio for Er (III)-complexes range from 0.814 to 0.998 in different metal-ligand stoichiometry, respectively. These values indicate co-ordination through oxygen in all the metal complexes. The values of the Judd-Ofelt Parameter,T_2, also used to estimate the photo luminescent property of the metal ion, higher the value of T_2 greater is the luminescence properties. The changes in values of T_λ parameters of the metal complexes indicate slight variation in stereo environment around central metal- ion. The values of the Judd-Ofelt parameter (T_λ) have been summarized in Table 3.

C. Bonding Parameters

*1) Nephelauxetic ratio (β):*InEr (III) complexes the nephelauxetic ratio (β) have been calculated using following equation(3)-

$$\beta = \nu_c / \nu_f \quad (3)$$

whereν_c and ν_f are energies (in cm^{-1}) of the hypersensitive transition in the complex and free-ion, respectively. For all the ternary complexes, the values of β are less than 1.0 which suggest that there is covalency. The values of β have been found in the range of 0.987 to 0.999.The values of nephelauxetic parameters, (β) have been evaluated and collected in Table-2.

2) Covalency Parameters ($b^{1/2}$): It also throws light on nature of metal-ligand bonding and its positive value indicates covalency. This is a measure of the amount of 4*f* –metal and ligand orbitals mixing in a complex. The bonding parameter ($b^{1/2}$) is also related to nephelauxetic ratio (β) by the equation (4)-

$$b^{1/2} = [{}^1/_2 (1-\beta)]^{1/2} \quad (4)$$

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The minimum and maximum values of $b^{1/2}$ have been found to be 0.104 to 0.078 respectively. This indicates the metal ligand interaction is not merely an ionic but there is a mixing of metal and ligands orbitals and hence covalent nature of metal-ligand bond (Ln-O) may be concluded [14]. The values of bonding parameters, ($b^{1/2}$) have been evaluated and are collected in Table-2.

IV. CONCLUSIONS

The interaction of Er (III) ions with crown ethers and amino acids is not just ionic but the various parameters evaluated advocate covalency in the bonding. In case of both the Er (III) metal ion complexes, the absorption was highest for 1:3:2 metal ligand stoichiometric ratio. On the basis of bonding parameter the order of covalency of the Er (III) metal ion complexes with these ligand is follows-

CE-GY > CE-AL > CE-AR > CB-GY > CB-AL > CB-AR > CD-GY > CD-AL > CD-AR.

The complexation and covalency have been related to spectral intensity i.e. oscillator strength. The metal-ligand stoichiometry affects the oscillator strength; higher the value of oscillator strength, higher will be complexation and covalency. This is in an agreement with earlier findings [15-18]

V. ACKNOWLEDGEMENTS

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Table –1 The values of Oscillator strength, Energies (in cm^{-1}) & wave-lengths of the various bands of Er (III) complexes of CE, CB or CD (L_1) with AL, GY or AR (L_2) in 1:3:2 metal-ligand stoichiometry.

Crown ether (L_1)	Amino acid (L_2)	Wave-length / Oscillator Strength / Energy	Levels							
			$^2G_{7/2}$	$^4G_{9/2}$	$^4G_{11/2}{}^*$	$^2H_{9/2}$	$^4F_{3/2}$	$^4F_{5/2}$	$^4F_{7/2}$	$^2H_{11/2}$
CE	β-Alanine	*λmax(nm)*	355.1	363.1	381.9	405.2	442.2	449.3	486.0	521.6
		Pexp×10⁶	0.631	1.814	8.061	0.931	0.516	0.905	1.668	2.870
		Pcalx10⁶	0.085	0.690	6.290	0.481	0.205	0.357	1.149	3.695
		Eexp(cm^{-1})	28144.09	27555.51	26532.34	24713.45	22672.75	22260.06	20564.43	19178.88
		Ecal(cm^{-1})	28151.23	27432.56	26670.04	24705.41	22532.15	22203.03	20508.97	19375.56
	Glycine	*λmax(nm)*	355.0	363.2	382.0	405.3	442.1	449.3	486.2	521.8
		Pexp×10⁶	0.658	1.835	8.073	0.957	0.523	0.927	1.683	2.891
		Pcalx10⁶	0.146	0.710	6.321	0.506	0.223	0.373	1.165	3.721
		Eexp(cm^{-1})	28140.35	27537.71	26515.33	24710.15	22655.52	22251.79	20545.87	19170.07
		Ecal(cm^{-1})	28150.98	27430.09	26671.71	24698.87	22534.41	22201.64	20500.44	19364.91
	L-Arginine	*λmax(nm)*	355.5	364.2	381.8	405.5	441.1	449.3	486.0	521.4
		Pexp×10⁶	0.585	1.493	8.001	0.653	0.329	0.597	1.609	2.431
		Pcalx10⁶	0.061	0.656	5.843	0.441	0.167	0.301	1.141	3.610
		Eexp(cm^{-1})	28129.21	27422.20	26658.90	24715.65	22515.55	22197.07	20495.55	19177.37
		Ecal(cm^{-1})	28141.02	27325.72	26608.90	24605.65	22405.55	22095.91	20465.67	19377.76
CB	β-Alanine	*λmax(nm)*	355.1	363.1	379.7	405.2	442.2	449.3	486.0	521.6
		Pexp×10⁶	0.615	1.801	8.049	0.921	0.501	0.896	1.651	2.854
		Pcalx10⁶	0.071	0.661	6.180	0.421	0.196	0.341	1.121	3.513
		Eexp(cm^{-1})	28122.09	27529.54	26528.78	24665.85	22630.31	22272.72	20572.24	19185.81
		Ecal(cm^{-1})	28115.38	27411.36	26662.26	24682.76	22532.54	22219.74	20517.17	19377.74
	Glycine	*λmax(nm)*	355.6	363.5	379.8	405.2	442.2	449.3	486.3	521.5

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Crown ether (L_1)	Amino acid (L_2)	Wave-length / Oscillator Strength / Energy	Levels							
			$^2G_{7/2}$	$^4G_{9/2}$	$^4G_{11/2}{}^*$	$^2H_{9/2}$	$^4F_{3/2}$	$^4F_{5/2}$	$^4F_{7/2}$	$^2H_{11/2}$
		Pexp×10⁶	0.621	1.810	8.053	0.931	0.511	0.903	1.670	2.870
		Pcalx10⁶	0.129	0.676	6.291	0.446	0.213	0.372	1.603	3.710
		Eexp(cm⁻¹)	28129.80	27533.05	26514.67	24675.57	22648.42	22245.56	20552.25	19184.46
		Ecal(cm⁻¹)	28122.09	27416.13	26662.27	24682.22	22538.62	22217.92	20514.16	19370.07
	L-Arginine	*λmax(nm)*	355.6	363.5	379.6	405.0	441.2	449.3	486.4	521.5
		Pexp×10⁶	0.579	1.384	7.843	0.591	0.301	0.487	1.583	2.381
		Pcalx10⁶	0.051	0.551	4.971	0.398	0.154	0.296	1.150	3.590
		Eexp(cm⁻¹)	28095.17	27489.80	26513.47	24700.77	22675.15	22256.06	20552.23	19175.55
		Ecal(cm⁻¹)	28121.01	27398.09	26670.61	24688.62	22547.92	22212.19	20523.21	19358.08
CD	β-Alanine	*λmax(nm)*	355.5	363.1	378.5	405.0	441.2	449.4	486.7	521.6
		Pexp×10⁶	0.403	1.253	7.091	0.659	0.280	0.738	1.223	2.200
		Pcalx10⁶	0.743	0.607	5.357	0.380	0.170	0.301	1.036	3.251
		Eexp(cm⁻¹)	28109.77	27509.8	26472.75	24695.54	22640.19	22262.21	20551.31	19180.60
		Ecal(cm⁻¹)	28111.67	27410.56	26645.61	24682.28	22518.75	22215.22	20514.42	19358.81
	Glycine	*λmax(nm)*	355.4	363.6	378.6	405.2	441.2	449.3	486.5	521.8
		Pexp×10⁶	0.418	1.275	7.131	0.671	0.295	0.755	1.246	2.221
		Pcalx10⁶	0.868	0.635	5.532	0.394	0.186	0.328	1.041	3.278
		Eexp(cm⁻¹)	28065.16	27424.54	26485.76	24654.42	22648.73	22223.54	20435.17	19186.68
		Ecal(cm⁻¹)	28077.08	27364.72	26612.14	24648.67	22515.16	22202.74	20492.27	19195.92
	L-Arginine	*λmax(nm)*	355.1	363.3	378.4	405.0	442.6	449.6	486.4	521.4
		Pexp×10⁶	0.367	1.005	6.541	0.609	0.224	0.519	1.185	2.010
		Pcalx10⁶	0.708	0.505	4.938	0.371	0.169	0.295	1.001	3.000
		Eexp(cm⁻¹)	28093.03	27482.28	26531.31	24682.23	22627.72	22267.71	20541.41	19221.38

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Crown ether (L_1)	Amino acid (L_2)	Wave-length / Oscillator Strength / Energy	Levels							
			$^2G_{7/2}$	$^4G_{9/2}$	$^4G_{11/2}{}^*$	$^2H_{9/2}$	$^4F_{3/2}$	$^4F_{5/2}$	$^4F_{7/2}$	$^2H_{11/2}$
		Ecal(cm^{-1})	28102.16	27380.12	26644.47	24676.92	22525.62	22225.15	20507.17	19355.15

Table- 2 Computed values of various spectral parameters (F_k, ζ_{4f}, E^k, β and $b^{1/2}$) of Er (III) complexes of CE, CB or CD (L_1) with AL, GY or AR (L_2), respectively, in 1:3:2 metal-ligand stoichiometry.

Ligand (L_1)	Ligand (L_2)	Slater-Condon Parameters (F_k)			Landé Parameter (ζ_{4f})	Racah Parameters (E^k)			Nephelauxetic ratio (β)	Co-valence Parameter ($b^{1/2}$)
		F_2	F_4	F_6		E^1	E^2	E^3		
CE	AL	435.70	65.52	7.55	2439.40	6795.18	33.31	622.40	0.988	0.077
	GY	435.80	66.54	7.75	2439.40	6796.20	33.61	623.40	0.987	0.078
	AR	435.80	65.54	7.75	2438.30	6795.10	32.60	623.40	0.988	0.076
CB	AL	434.60	65.66	7.73	2470.90	6791.80	32.44	620.90	0.993	0.055
	GY	434.80	65.68	7.75	2471.10	6792.00	32.46	621.10	0.993	0.057
	AR	434.50	65.65	7.72	2470.80	6791.70	32.43	620.80	0.994	0.054
CD	AL	438.90	64.88	7.83	2456.20	6819.30	33.22	623.70	0.996	0.039
	GY	438.40	65.96	7.83	2458.20	6817.30	34.14	624.30	0.996	0.040
	AR	439.90	64.83	7.94	2458.10	6854.60	33.45	623.00	0.997	0.037

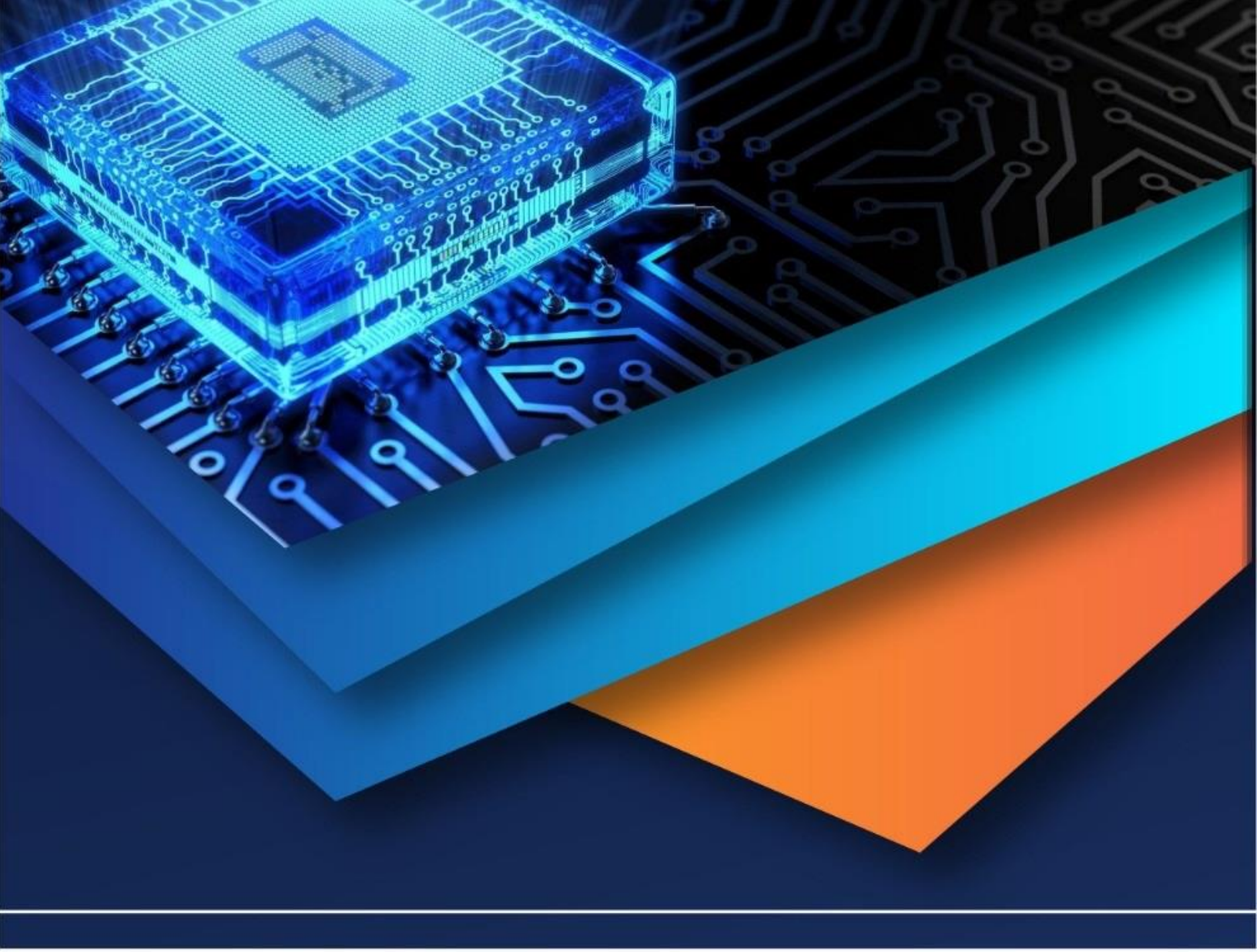
Table- 3 Computed values of Judd-OfeltParameter (T_λ) for Er(III) complexes of CE, CB or CD (L_1) with AL, GY or AR (L_2), respectively, in 1:3:2 stoichiometry.

Crown ether (L_1)	Amino acid (L_2)	Parameters $T_\lambda \times 10^9$			
		T_2	T_4	T_6	T_4/T_6

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CE	AL	0.233	0.094	0.113	0.835
	GY	0.194	0.096	0.112	0.856
	AR	0.238	0.095	0.115	0.826
CB	AL	0.213	0.094	0.110	0.857
	GY	0.238	0.095	0.085	0.890
	AR	0.164	0.075	0.115	0.828
CD	AL	0.194	0.104	0.104	0.998
	GY	0.214	0.124	0.124	0.998
	AR	0.186	0.093	0.114	0.814

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