



Research Article

Calculation of Shifting in Energy Levels for Ln^{3+} (Pr^{3+} , Nd^{3+}) Complex's with Hetero cyclic Ligands in Solution state by using Optical Absorption Spectra

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Abstract: The absorption spectra of Ln^{3+} (Pr^{3+} and Nd^{3+}) were investigated in UV visible regions at room temperature. Theoretical analysis of the results including the effects of configuration interaction is discussed. Good correlation between calculated and observed free-ion level energies established. Comparison of the levels observed in the solution with reported gaseous free-ion levels indicated that there is little change in the J -level structure in the $4f^n$ configuration. Excellent agreement between observed and calculated energies is obtained.

Keywords: Hetero Cyclic Ligands, Optical Absorption Spectra, Energy Levels, UV Visible

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Conflict of interest: None

Introduction

The tripositive rare earths ions exhibit sharp electronic absorption spectra which originating from the intra $4f \rightarrow 4f$ transitions of electrons [1]. Upon complexation, the absorption spectra of aquated rare-earth ions undergo key alterations, including the splitting of specific bands into multiple Stark components, subtle bathochromic shifts (toward longer wavelengths), and variations in molar absorptivity. These modifications arise from fluctuations in local crystal field strength and coordination symmetry. Consequently, electronic absorption spectra serve as a sensitive probe for investigating molecular geometry, coordination numbers, and microenvironment variations of lanthanide complexes in solution. However, the results for lanthanide ions are useful when contrasted with a transition [2-4].

For lanthanide ions, the perturbation terms in decreasing order of energy are:

Inter-electronic repulsions > Spin-orbit coupling > Crystal field

Optical absorption spectra cannot be used to determine the kind of bonding in rare earth complexes because light absorption of ligands has no effect on the electronic transition in the well-shielded 4f orbitals of rare earth ions. Nevertheless, the wavelength shift shows that 4f orbitals are involved in the formation of incredibly weak covalent bonds despite its minuscule magnitude. Electronic absorption spectroscopy remains a vital characterization tool, as interpretative frameworks grounded in Crystal Field Theory (CFT) and Ligand Field Theory (LFT) enable the elucidation of electronic structure, coordination geometry, and metal-ligand interactions.

Method:

It is known that 4f-4f transitions cause the absorption spectra of lanthanide ions in the visible and near-IR regions (1). The electrostatic and magnetic interactions between 4f electrons can be thought of as the source of the energy level structure of the $4f^n$ configuration. These interactions can be expressed in terms of Slater-Condon (F_k), Lande (ζ_{4f}) and Racah (E^k) Parameters.

Slater- condon- Lande Equation: The energy of the j^{th} electronic level (E_j) can be evaluated by expressing it as a Taylor series expansion in terms of the Slater-Condon electrostatic interaction parameters (F_k , where $k = 2, 4, 6$) and the Landé spin-orbit coupling constant (ζ_{4f}). Under the first-order Taylor approximation, the energy E_j of a given J -level is expressed as:

$$E_j(F_k, \zeta_{4f}) = E_{oj}(F_k^0, \zeta_{4f}^0) + \sum (\partial E_j / \partial F_k) \Delta F_k + (\partial E_j / \partial \zeta_{4f}) \Delta \zeta_{4f} \quad (1)$$

$k = 2, 4, 6$

$$E_{\text{obs}} = E_{oj} + (\partial E_j / \partial F_2) \Delta F_2 + (\partial E_j / \partial F_4) \Delta F_4 + (\partial E_j / \partial F_6) \Delta F_6 + (\partial E_j / \partial \zeta_{4f}) \Delta \zeta_{4f} \quad (2)$$

$$E_{\text{obs}} - E_{oj} = (\partial E_j / \partial F_2) \Delta F_2 + (\partial E_j / \partial F_4) \Delta F_4 + (\partial E_j / \partial F_6) \Delta F_6 + (\partial E_j / \partial \zeta_{4f}) \Delta \zeta_{4f} \quad (3)$$

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

Where, Energy of Zero-order j^{th} level is E_{oj}

Energy of j^{th} level is E_j

$\Delta \zeta_{4f}$ - Slight deviation in the Lande parameters

ΔF_k - Slight deviation in the Slater-Condon parameters

$(\partial E_j / \partial F_k)$ - Partial differentiation with respect to F_k

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

The values of ΔF_k and $\Delta \zeta_{4f}$ may be evaluated using observed energy values (E_j), reported result of zero-order energies (E_{oj}) and partial derivatives $(\partial E_j / \partial F_k)$ and $(\partial E_j / \partial \zeta_{4f})$ by partial - multiple regression method [5-11].

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

$$F_k = F_k^0 + \Delta F_k \quad (5)$$

$$\zeta_{4f} = \zeta_{4f}^0 + \Delta \zeta_{4f} \quad (6)$$

Where, $\Delta F_k \ll F_k^0$, $\Delta \zeta_{4f} \ll \zeta_{4f}^0$ and F_k^0 and ζ_{4f}^0 are the zero -order values by Wong (3).

(b) R.M.S. Deviations (Energy):

The calculated values of the parameters have been used to estimate the energies E_j of the electronic states. The correspondence between calculated (E_{cal}) and observed (E_{obs}) energy levels was measured through calculation the root-mean-square deviation (σ) according to the relation:-

$$\sigma = \{\sum (E_{\text{cal}} - E_{\text{obs}})^2 / N\}^{1/2} \quad (7)$$

Where, N is the number of energy levels that are fitted

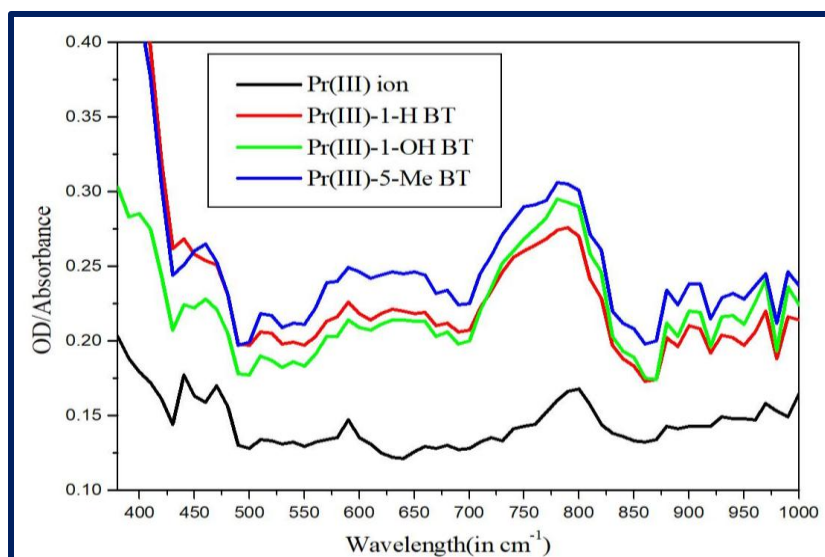


Figure 1: Electronic Absorption Spectra of Pr(III) ion and Pr(III)-1-H BT, Pr(III)-1-OH BT, Pr(III)-5-Me BT system in alcoholic: aqua solution

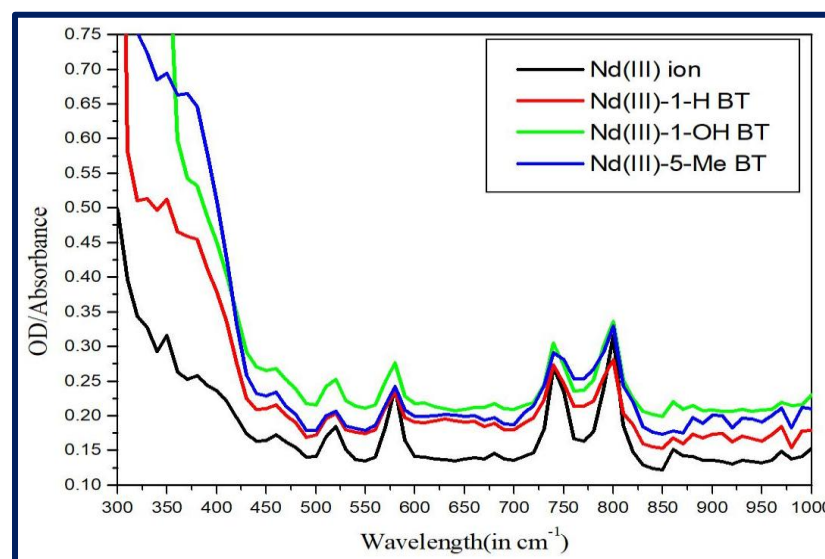


Figure 2: Electronic Absorption Spectra of Nd(III) ion and Nd(III)-1-H BT, Nd(III)-1-OH BT, Nd(III)-5-Me BT system in alcoholic: aqua solution

Table 1: Experimental and Computed value of Energy (cm^{-1}) for various energy level of Pr(III)-1-H BT, Pr(III)-1-OH BT, Pr(III)-5-Me BT system in alcoholic: aqua solution

S.N.	System Energy Level	Pr(III)-1-H BT			Pr(III)-1-OH BT			Pr(III)-5-Me BT		
		$E_{cal.}$	$E_{exp.}$	ΔE	$E_{cal.}$	$E_{exp.}$	ΔE	$E_{cal.}$	$E_{exp.}$	ΔE
1.	$^3H_4 \rightarrow ^3P_2$	22447.3	22446.7	0.60	22472.5	22471.9	0.60	22371.9	22371.36	0.54
2.	$^3H_4 \rightarrow ^3P_1$	21276.7	21276.6	0.10	21344.8	21344.7	0.10	21254.1	21253.99	0.11
3.	$^3H_4 \rightarrow ^3P_0$	20681.5	20682.5	-1.00	20703.1	20703.9	-0.80	20660.1	20661.16	-1.06
4.	$^3H_4 \rightarrow ^1D_2$	16920.6	16920.5	0.10	16949.3	16949.2	0.10	16906.4	16906.17	0.23
5.	r.m.s. (σ) dev.($\pm$)		0.56			0.52			0.57	

Table 2: Experimental and Computed value of Energy (cm^{-1}) for various energy level of Pr(III)-1-H BT, Pr(III)-1-OH BT, Pr(III)-5-Me BT system in micellar (TX-100) solution

S.N.	System Energy Level	Pr(III)-1-H BT			Pr(III)-1-OH BT			Pr(III)-5-Me BT		
		$E_{cal.}$	$E_{exp.}$	ΔE	$E_{cal.}$	$E_{exp.}$	ΔE	$E_{cal.}$	$E_{exp.}$	ΔE
1.	$^3\text{H}_4 \rightarrow ^3\text{P}_2$	22422.2	22421.5	0.70	22397.0	22396.4	0.60	22222.6	22222.2	0.40
2.	$^3\text{H}_4 \rightarrow ^3\text{P}_1$	21276.7	21276.6	0.10	21276.7	21276.6	0.10	21254.0	21253.9	0.10
3.	$^3\text{H}_4 \rightarrow ^3\text{P}_0$	20617.8	20618.6	-0.80	20702.8	20703.9	-1.10	20638.9	20639.8	-0.90
4.	$^3\text{H}_4 \rightarrow ^1\text{D}_2$	16891.9	16891.8	0.10	16906.4	16906.2	0.20	16906.5	16906.8	-0.30
5.	r.m.s.(o) dev. ($\pm$)		0.52			0.65			0.56	

Table 3: Experimental and Computed value of Energy (cm^{-1}) for various energy level of Pr(III)-1-H BT, Pr(III)-1-OH BT, Pr(III)-5-Me BT system in micellar (SDS) solution

S.N.	System Energy Level	Pr(III)-1-H BT			Pr(III)-1-OH BT			Pr(III)-5-Me BT		
		$E_{cal.}$	$E_{exp.}$	ΔE	$E_{cal.}$	$E_{exp.}$	ΔE	$E_{cal.}$	$E_{exp.}$	ΔE
1.	$^3\text{H}_4 \rightarrow ^3\text{P}_2$	22497.7	22497.1	0.60	22497.9	22497.1	0.80	22396.9	22396.4	0.50
2.	$^3\text{H}_4 \rightarrow ^3\text{P}_1$	21254.1	21253.9	0.20	21344.8	21344.7	0.10	21299.3	21299.3	0.00
3.	$^3\text{H}_4 \rightarrow ^3\text{P}_0$	20681.8	20682.5	-0.70	20660.4	20661.2	-0.80	20596.8	20597.3	-0.50
4.	$^3\text{H}_4 \rightarrow ^1\text{D}_2$	16963.6	16963.5	0.10	16920.5	16920.5	0.00	16934.8	16934.8	0.00
5.	r.m.s. (o) dev. ($\pm$)		0.46			0.51			0.37	

Table 4: Experimental and Computed value of Energy (cm^{-1}) for various energy level of Pr(III)-1-H BT, Pr(III)-1-OH BT, Pr(III)-5-Me BT system in micellar (HTAB) solution

S.N.	System Energy Level	Pr(III)-1-H BT			Pr(III)-1-OH BT			Pr(III)-5-Me BT		
		$E_{cal.}$	$E_{exp.}$	ΔE	$E_{cal.}$	$E_{exp.}$	ΔE	$E_{cal.}$	$E_{exp.}$	ΔE
1.	$^3\text{H}_4 \rightarrow ^3\text{P}_2$	22462.5	22461.8	0.70	22447.3	22446.7	0.60	22222.6	22222.2	0.40
2.	$^3\text{H}_4 \rightarrow ^3\text{P}_1$	21312.9	21312.9	0.00	21299.3	21299.3	0.00	21254.0	21253.9	0.10
3.	$^3\text{H}_4 \rightarrow ^3\text{P}_0$	20681.6	20682.5	-0.90	20681.6	20682.5	-0.90	20638.9	20639.8	-0.90
4.	$^3\text{H}_4 \rightarrow ^1\text{D}_2$	16906.3	16906.3	0.00	16920.6	16920.5	0.10	16906.5	16906.2	0.30
5.	r.m.s. (o) dev. ($\pm$)		0.58			0.56			0.56	

Table 5: Experimental and Computed value of Energy (cm^{-1}) for various energy level of Nd(III)-1-H BT, Nd(III)-1-OH BT, Nd(III)-5-Me BT system in alcoholic: aqua solution

S.N	System Energy Level	Nd(III)-1-H BT			Nd(III)-1-OH BT			Nd(III)-5-Me BT		
		$E_{cal.}$	$E_{exp.}$	ΔE	$E_{cal.}$	$E_{exp.}$	ΔE	$E_{cal.}$	$E_{exp.}$	ΔE
1.	$^4\text{I}_{9/2} \rightarrow ^4\text{D}_{1/2}$	28669.8	28557.5	112.30	28668.4	28571.4	97.00	28669.4	28568.1	101.30
2.	$^4\text{I}_{9/2} \rightarrow ^4\text{G}_{11/2}$	21165.6	21746.6	581.00	21165.8	21723.5	557.70	21168.6	21734.8	-566.20
3.	$^4\text{I}_{9/2} \rightarrow ^4\text{G}_{9/2}$	18548.4	19227.4	679.00	18548.6	19236.6	688.00	18549.6	19236.3	-686.70
4.	$^4\text{I}_{9/2} \rightarrow ^4\text{G}_{7/2}$	18237.5	17239.8	997.70	18237.7	17239.0	998.70	18238.6	17237.8	1000.80
5.	$^4\text{I}_{9/2} \rightarrow ^4\text{F}_{9/2}$	14928.8	14700.4	228.40	14929.5	14706.7	222.80	14933.2	14707.8	225.40
6.	$^4\text{I}_{9/2} \rightarrow ^4\text{F}_{7/2}$	13407.3	13514.4	107.10	13407.2	13512.4	105.20	13409.2	13516.8	-107.60
7.	$^4\text{I}_{9/2} \rightarrow ^2\text{H}_{9/2}$	12470.2	12501.0	-30.80	12471.0	12501.5	-30.50	12473.0	12503.7	-30.70
8.	$^4\text{I}_{9/2} \rightarrow ^4\text{F}_{3/2}$	11602.3	11626.8	-24.50	11601.7	11625.3	-23.60	11602.5	11625.4	-22.90
9.	r.m.s. (o) dev. ($\pm$)		483.72			481.35			483.20	

Table 6: Experimental and Computed value of Energy (cm⁻¹) for various energy level of Nd (III)-1-H BT, Nd(III)-1-OH BT, Nd(III)-5-Me BT system in micelle (TX-100) solution

S.N	System Energy Level	Nd(III)-1-H BT			Nd(III)-1-OH BT			Nd(III)-5-Me BT		
		<i>E_{cal.}</i>	<i>E_{exp.}</i>	ΔE	<i>E_{cal.}</i>	<i>E_{exp.}</i>	ΔE	<i>E_{cal.}</i>	<i>E_{exp.}</i>	ΔE
1.	⁴ I _{9/2} → ⁴ D _{1/2}	28662.0	28547.8	114.20	28666.3	28571.4	94.90	28675.2	28578.8	96.40
2.	⁴ I _{9/2} → ⁴ G _{11/2}	21169.8	21730.6	-560.80	21169.8	21741.0	-571.20	21166.4	21741.5	-575.10
3.	⁴ I _{9/2} → ⁴ G _{9/2}	18544.6	19233.7	-689.10	18549.0	19235.9	-686.90	18549.4	19225.6	-676.20
4.	⁴ I _{9/2} → ⁴ G _{7/2}	18230.8	17233.0	997.80	18237.0	17233.3	1003.70	18239.2	17246.1	993.10
5.	⁴ I _{9/2} → ⁴ F _{9/2}	14935.8	14713.0	222.80	14935.0	14710.2	224.80	14928.5	14704.6	223.90
6.	⁴ I _{9/2} → ⁴ F _{7/2}	13410.1	13512.2	-102.10	13409.6	13512.0	-102.40	13408.5	13507.8	-99.30
7.	⁴ I _{9/2} → ² H _{9/2}	12461.4	12491.9	-30.50	12470.5	12501.2	-30.70	12471.3	12501.9	-30.60
8.	⁴ I _{9/2} → ⁴ F _{3/2}	11600.0	11630.5	-30.50	11601.2	11624.7	-23.50	11604.8	11628.7	-23.90
9.	r.m.s. (σ) dev. (±)		482.16			484.37			480.22	

Table 7: Experimental and Computed value of Energy (cm⁻¹) for various energy level of Nd(III)-1-H BT, Nd(III)-1-OH BT, Nd(III)-5-Me BT system in micelle (SDS) solution

S.N	System Energy Level	Nd(III)-1-H BT			Nd(III)-1-OH BT			Nd(III)-5-Me BT		
		<i>E_{cal.}</i>	<i>E_{exp.}</i>	ΔE	<i>E_{cal.}</i>	<i>E_{exp.}</i>	ΔE	<i>E_{cal.}</i>	<i>E_{exp.}</i>	ΔE
1.	⁴ I _{9/2} → ⁴ D _{1/2}	28674.2	28564.9	109.30	28651.2	28571.4	79.80	28661.2	28522.5	138.70
2.	⁴ I _{9/2} → ⁴ G _{11/2}	21164.6	21741.0	-576.40	21091.5	21746.2	-654.70	21164.4	21736.7	-572.30
3.	⁴ I _{9/2} → ⁴ G _{9/2}	18554.2	19233.3	-679.10	18535.8	19230.0	-694.20	18547.1	19223.3	-676.20
4.	⁴ I _{9/2} → ⁴ G _{7/2}	18242.9	17246.4	996.50	18294.4	17238.1	1056.30	18235.9	17249.7	986.20
5.	⁴ I _{9/2} → ⁴ F _{9/2}	14920.3	14692.0	228.30	14959.0	14707.6	251.40	14930.2	14703.0	227.20
6.	⁴ I _{9/2} → ⁴ F _{7/2}	13403.9	13514.6	-110.70	13387.2	13510.5	-123.30	13405.6	13514.7	-109.10
7.	⁴ I _{9/2} → ² H _{9/2}	12465.5	12496.4	-30.90	12789.0	12822.6	-33.60	12471.3	12501.8	-30.50
8.	⁴ I _{9/2} → ⁴ F _{3/2}	11601.0	11623.1	-22.10	11621.9	11625.0	-3.10	11598.5	11630.2	-31.70
9.	r.m.s. (σ) dev. (±)		482.71			513.85			479.85	

Table 8: Experimental and Computed value of Energy (cm⁻¹) for various energy level of Nd (III)-1-H BT, Nd(III)-1-OH BT, Nd(III)-5-Me BT system in micelle (HTAB) solution

S.N	System Energy Level	Nd(III)-1-H BT			Nd(III)-1-OH BT			Nd(III)-5-Me BT		
		<i>E_{cal.}</i>	<i>E_{exp.}</i>	ΔE	<i>E_{cal.}</i>	<i>E_{exp.}</i>	ΔE	<i>E_{cal.}</i>	<i>E_{exp.}</i>	ΔE
1.	$^4I_{9/2} \rightarrow ^4D_{1/2}$	28657.7	28544.5	113.20	28673.2	28571.4	101.80	28675.3	28578.8	96.50
2.	$^4I_{9/2} \rightarrow ^4G_{11/2}$	21165.6	21731.1	-565.50	21165.7	21749.0	-583.30	21166.4	21741.5	-575.10
3.	$^4I_{9/2} \rightarrow ^4G_{9/2}$	18543.9	19226.7	-682.80	18554.8	19234.8	-680.00	18549.4	19225.6	-676.20
4.	$^4I_{9/2} \rightarrow ^4G_{7/2}$	18231.4	17237.5	993.90	18244.0	17243.4	1000.60	18239.2	17246.1	993.10
5.	$^4I_{9/2} \rightarrow ^4F_{9/2}$	14933.5	14708.9	224.60	14923.6	14696.5	227.10	14928.5	14704.6	223.90
6.	$^4I_{9/2} \rightarrow ^4F_{7/2}$	13407.2	13512.9	-105.70	13404.9	13506.7	-101.80	13408.5	13507.8	-99.30
7.	$^4I_{9/2} \rightarrow ^2H_{9/2}$	12467.1	12497.7	-30.60	12470.8	12501.7	-30.90	12471.3	12501.9	-30.60
8.	$^4I_{9/2} \rightarrow ^4F_{3/2}$	11598.0	11625.0	-27.00	11601.2	11625.3	-24.10	11604.8	11628.7	-23.90
9.	r.m.s. (o) dev. (±)		480.89			484.46			480.22	

Optical absorption spectra of Pr³⁺ system:- Four electronic absorption bands ($^3H_4 \rightarrow ^3P_2$, $^3H_4 \rightarrow ^3P_1$, $^3H_4 \rightarrow ^3P_0$ and $^3H_4 \rightarrow ^1D_2$) for Pr³⁺ system with derivatives of benzotriazole in doping of viz:-1-H BT, 1-OH BT, 5-Me BT in the medium of alcohol – water (1:1) and micellar (TX-100) have been obtained in the region 400 nm to 900 nm. All eight systems spectra have been shown in figures 1.0 for Pr(III) doped system with benzotriazole derivatives viz:- 1-H BT, 1-OH BT, 5-Me BT (12-15).

Optical absorption spectra of Nd³⁺ system:- Eight electronic absorption bands like $^4I_{9/2} \rightarrow ^4D_{1/2}$, $^4I_{9/2} \rightarrow ^4G_{11/2}$, $^4I_{9/2} \rightarrow ^4G_{9/2}$, $^4I_{9/2} \rightarrow ^4G_{7/2}$, $^4I_{9/2} \rightarrow ^4F_{9/2}$, $^4I_{9/2} \rightarrow ^4F_{7/2}$, $^4I_{9/2} \rightarrow ^4F_{7/2}$, and $^4I_{9/2} \rightarrow ^4F_{3/2}$ for Nd³⁺ with derivatives of benzotriazole in doping of viz:-1-H BT, 1-OH BT, 5-Me BT in the medium of alcohol – water (1:1) and micellar (TX-100) have been obtained in the region 400 nm to 900 nm. Spectra of each of the eight systems has been shown in figures 2.0.

To evaluate oscillator strength with higher precision, the half bandwidth ($\nu_{1/2}$) was calculated by deconvoluting the experimental absorption bands into individual Gaussian components. This curve-fitting approach effectively isolated overlapping transitions, thereby improving the accuracy of the spectroscopic and Judd-Ofelt parameters derived.

Conclusion

For the Pr(III)-1H-benzotriazole complex in the alcoholic system, the calculated energy (*E_{cal}*) values remain practically identical across all observed electronic transitions.

For Pr(III)-1-OH BT in complex in the alcoholic system, the calculated energy (*E_{cal}*) values remain practically identical across all observed electronic transitions.

rms(o) dev. (±) is very small as for every system that is always same i.e. it vary from 0.58 to 0.61.2. For Pr(III) -1-H BT in micellar system *E_{cal}* is 22599.5 and *E_{exp}* is 22598.87 for $^3H_4 \rightarrow ^3P_1$ transition For Pr(III) -1-OH BT system in micellar medium *E_{cal}* is 22573.98 and *E_{exp}* is 22573.36 for $^3H_4 \rightarrow ^3P_1$ transition. For Pr(III) -5-Me BT in micellar system *E_{cal}* is 22548.62 and *E_{exp}* is 22547.91. In micellar system rms dev. (o±) is very small as for all systems For Nd(III) -1-H BT in alcoholic system *E_{cal}* and *E_{exp}* is nearby same with respect to all transition In micellar medium, For Nd(III) -1-H BT system *E_{cal}* and *E_{exp}* is nearby same with respect to all transition.

Theoretical Validation: Partial-multiple regression method is applying for Taylor series expansion (evaluating Slater-Condon parameters F_k and Landé parameter ζ_{4f}). It gives an accurate mathematical fit for experimental $4f \rightarrow 4f$ transition energies.

Perturbation Hierarchy: The spectral conduct confirms that electrostatic inter-electronic repulsions and spin-orbit coupling dominate over the weaker ligand crystal field effects:

Crystal Field, Spin-Orbit Coupling, Inter-Electronic Repulsions

Ligand Effect: Methyl substitution (5-Me BT) usually generates lower RMS energy deviations relative to unsubstituted (1-H BT) or hydroxyl-substituted (1-OH BT) ligands.

High Mathematical Precision: The application of the Slater-Condon (F_k) and Landé (ζ_{4f}) parameterization scheme via Taylor series expansion and partial-multiple regression demonstrates outstanding theoretical accuracy. The model yields exceptionally low RMS energy deviations (σ) for Pr^{3+} complexes (± 0.37 to $\pm 0.65 \text{ cm}^{-1}$), confirming that first-order energy approximations reliably predict experimental $4f \rightarrow 4f$ transition energies.

Microenvironment & Surfactant Modulation: Spectral fits vary based on the surfactant headgroup charge in micellar systems:

Anionic (SDS): Produces the tightest agreement between E_{cal} and E_{exp} (lowest σ values), suggesting enhanced structural rigidity and uniform local symmetry around the lanthanide core.

Cationic (HTAB) & Non-Ionic (TX-100): Display slightly higher RMS deviations, reflecting minor variations in local hydration shells and dielectric microenvironments.

Substituent Influence on Complexation: Structural modifications on the benzotriazole directly influence bonding strength and geometry. Electron-donating methyl substitution (5-Me BT) consistently yields lower RMS deviations and higher spectral reproducibility than unsubstituted (1-H BT) or hydroxyl-substituted (1-OH BT) analogs, pointing to superior complex stability.

Structural Applicability: Overall, electrical absorption spectroscopy used in combination with partial-multiple regression analysis serves as a sensitive probe for characterizing the solution-state coordination environments, local symmetries, and subtle covalent interactions in rare-earth heterocycle complexes]

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