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Spectrophotometric Characterisation of Doped Pr(III) Ion in Saturated Aqueous Solution of Some Pharmaceutical Compounds

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The stereo-environment of doped Pr(III) ion in saturated solution of some pharmaceutical organic compounds in aqueous media has been discussed on the basis of various electronic spectral parameters. The various electronic parameters, *viz.*, Judd-Ofelt intensity parameter, T_λ, Slater-Condon (F_k), Lande's (ζ_{4f}) intensity of hypersensitive band ($^3P_2$) and Racah's (E_k) as well as bonding parameter $b^{1/2}$ for Pr(III) ion doped in aqueous saturated solution of diphenhydramine, tripelennamine, chlorphenaramine, promethazine, terfinadine, naproxen, fenoprofen, flurbiprofen, oxaprozin, ketoprofen a..d ibuprofen.

INTRODUCTION

In the present discussion the study has been made on the basis of utility of some lanthanide substituted pharmaceutical compounds, owing to their immense medicinal application[1–3], on the ground of Judd-Ofelt and Slater-Condon theory. Since in the field of science and technology the doped study of certain system finds immense application[4–13], therefore, on the basis of Judd-Ofelt[14–17] intensity as well as other electronic spectral parameter's, a correlation of f ↔ f transition for Pr(III) ion doped in saturated solution of some pharmaceutical compounds and the stereo-environment around Pr(III) ion has been attempted. A saturated solution in aqueous media has been made by dissolving diphenhydramine, tripelennamine, chlorphenaramine, promethazine, terfinadine, naproxen, fenoprofen, flurbiprofen, oxaprozin, ketoprofen and ibuprofen at room temperature (30 ± 2°C) and a constant amount of Pr(III) chloride has been added to each of the solutions. Characterisation of some of the electronic parameters for Pr(III) ion doped in saturated aqueous solution of these compounds was made spectrophotometrically. On the basis that Pr(III) ion yields four bonds in visible region, *viz.*, $^3P_2$, $^3P_1$, $^3P_0$ and $^1D_2$ and the change in the intensity of these bands is indicated by red shift caused by the change coordination environment around the ion resulting from $f \leftrightarrow f$ transition in lanthanides.

EXPERIMENTAL

The various saturated solutions[18–23] of diphenhydramine, tripelennamine, chlorphenaramine, promethazine, terfinadine, naproxen, fenoprofen, flurbiprofen, oxaprozin, ketoprofen and ibuprofen of I.P. grade in aqueous media were prepared at room temperature ($30 \pm 2°C$) and 0.14 M of $PrCl_3 \cdot 6H_2O$ (99.9% purity supplied by India Rare Earth's Udyogmandalam, Kerala) had been added to each of the solutions. The solution spectra of these systems were recorded by using standard spectrophotometer[24–29] (Spectronic-20) in the visible region. The calculation for various electronic parameters was made by computerized statistical method reported earlier.[26–29]

RESULTS AND DISCUSSION

The computed values of various parameters have been given in Tables 1 and 2. The present study shows that the $f \leftrightarrow f$ transition resulting from spin orbit interaction in Pr(III) is due to interaction with the ligand present in the saturated solution are remarkabley manifested in terms of change in the energy of various electronic parameters. The decrease in computed values of spin orbit interaction parameter (ζ_{4f}), Oscillator strength of $^3P_2$ band, Judd-Ofelt parameter (T_λ) and Slater-Condon parameter (F_k) in comparison to free ion values clearly reflects symmetry change around the metal ion in the solution. The T_4/T_6 ratio reflects the change in stereo-environment around the metal ion present in the solution and thereby change in coordination number. Therefore, the change in the surrounding evironment around the metal ion involving the suitable interaction between the metal ion and ligand has been well characterized by decrease in the various inter-electronic repulsions and spin orbit interactions.

The parametric values provide useful information regarding the coordination behaviour of Pr(III) ion. The coordination behaviour varies as the change in ratio of T_4/T_6 takes place. The similar values indicate the similar stereo-environment around Pr(III) due to solute-interaction present in the solution.

The values of Slater-Condon parameter (F_K) in the present system decrease from free ion value and show close similarity whereas Lande's parameter (ζ_{4f}) which shows spin-orbit intraction has been found to show much variation. This shows that spin-orbit interactions in $f \leftrightarrow f$ transition are much more affected in comparison to inter-electronic interaction. The intensity of hypersensitivity band also shows similar trend.

The study provides useful information regarding stereo-environment around Pr(III) ion as significantly exhibited by T_4/T_6 ratio value. The nephelauxetic ratio as indicated by the values of $b^{1/2}$ also reflects some bonding character in the form of change in stereo-environment around the central metal ion.

The various other electronic parameters reported in the tables have their usual significance as reported earlier by one of the authors (P.R. Bhati)[26–28].

TABLE-1

COMPUTED VALUES OF ENERGY (cm^{-1}) OF OSCILLATOR STRENGTH T_λ AND T_4/T_6 FOR Pr(III) ION DOPED IN AQUEOUS SATURATED SOLUTION OF VARIOUS PHARMACEUTICAL ORGANIC COMPOUNDS

Compounds	$^3P_0 \times 10^{-6}$		$^3P_1 \times 10^{-6}$		$^3P_0 \times 10^{-6}$		$^1D_2 \times 10^{-6}$		$T_\lambda \times 10^{-10}$			T_4/T_6
	P_{exp}	P_{cal}	P_{exp}	P_{cal}	P_{exp}	P_{cal}	P_{exp}	P_{cal}	T_2	T_4	T_6	
Pr^{3+} : Diphenhydramine	23.5	23.5	10.90	10.90	2.48	2.47	6.70	6.70	–48.6	18.3	72.4	0.25
Pr^{3+} : Tripelennamine	29.6	29.6	8.22	8.22	3.35	3.34	4.53	4.53	–93.3	16.1	92.8	0.71
Pr^{3+} : Chlorphenaramine	55.8	55.8	33.10	33.10	8.58	8.54	16.30	16.30	–12.5	57.3	16.7	0.34
Pr^{3+} : Promethazine	14.5	14.5	5.24	5.24	1.72	1.71	3.81	3.81	–10.3	95.6	45.3	0.21
Pr^{3+} : Terfinadine	6.4	6.4	2.71	2.71	1.56	1.56	1.84	1.84	–73.1	58.8	19.4	0.30
Pr^{3+} : Naproxen	25.3	25.3	9.31	9.31	2.50	2.49	6.74	6.74	–16.6	16.3	79.5	0.20
Pr^{3+} : Fenoprofen	53.9	53.9	28.90	28.10	10.10	10.00	19.70	19.70	–31.1	67.2	21.7	0.31
Pr^{3+} : Flurbiprofen	13.6	13.6	5.77	5.77	2.23	2.22	3.79	3.79	–56.7	11.0	42.3	0.26
Pr^{3+} : Oxaprozin	15.3	15.3	6.08	6.08	1.77	1.77	3.78	3.78	–16.3	10.7	47.5	0.23
Pr^{3+} : Ketoprofen	37.45	37.45	23.34	23.31	7.49	7.45	10.30	10.03	–27.1	54.1	23.5	0.23
Pr^{3+} : Ibuprofen	17.7	17.7	7.45	7.45	2.76	2.75	5.09	5.09	–24.7	14.1	54.5	0.26

TABLE-2

COMPUTED VALUES OF F_k, ζ_{4f}, E_k, % $r\zeta_{4f}$, %r F_2, β and $b^{1/2}$ Pr(III) ION DOPED IN AQUEOUS SATURATED SOLUTIONS OF VARIOUS PHARMACEUTICAL ORGANIC COMPOUNDS

Compounds	F_2	F_4	F_6	% rF_2	ζ_{4f}	% $r\zeta_{4f}$	E^1	E^2	E^3	β	$b^{1/2}$
Pr^{3+} : Free ion	322.09	44.46	4.87	–	738.00	–	4729.00	24.78	478.13	–	–
Pr^{3+} : Diphenhydramine	312.35	43.12	4.71	3.02	668.57	9.77	4585.99	23.98	463.66	0.96978	0.12290
Pr^{3+} : Tripelennamine	310.52	42.86	4.69	3.59	675.11	8.89	4559.08	23.84	460.94	0.96409	0.13398
Pr^{3+} : Chlorphenaramine	309.31	42.70	4.67	3.96	701.34	5.35	4541.30	23.75	459.14	0.96033	0.14082
Pr^{3+} : Promethazine	309.19	42.68	4.67	4.00	711.93	3.92	4539.48	23.74	458.96	0.95995	0.14150
Pr^{3+} : Terfinadine	309.88	42.77	4.68	3.78	706.66	4.63	4549.70	23.79	459.99	0.96211	0.13763
Pr^{3+} : Naproxen	308.03	42.52	4.65	4.36	713.46	3.71	4522.54	23.65	457.25	0.95637	0.14769
Pr^{3+} : Fenoprofen	308.32	42.56	4.65	4.27	722.61	2.48	4526.83	23.67	457.68	0.95727	0.14615
Pr^{3+} : Flurbiprofen	308.42	42.57	4.66	4.24	710.52	4.11	4528.22	23.68	457.82	0.95757	0.14565
Pr^{3+} : Oxaprozin	316.84	43.74	4.78	1.62	598.44	19.23	4651.92	24.33	470.33	0.98373	0.09019
Pr^{3+} : Ketoprofen	309.19	42.68	4.67	4.00	711.93	3.92	4539.48	23.74	458.96	0.95995	0.14150
Pr^{3+} : Ibuprofen	310.55	42.87	4.69	3.58	675.00	8.90	4559.56	23.85	460.99	0.96419	0.13379

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