Asian Journal of Chemistry Vol. 13, No. 2 (2001), 803–805

NOTE

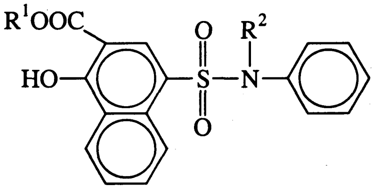
Electronic Spectral Studies on Nd^{3+} Doped Sulphonanilide Systems, Part-I

P.C. TATER, MS. ARYAMITRA PANDEY* and K.P. SONI
Rare Earth Research Laboratory, Department of Chemistry Government Dungar College
Bikaner-334 003 (Raj.), India

Six 3-carboalkoxy-4-hydroxy-N-alkylnaphthalene-1-sulphonanilide (where alkoxy = methoxy, ethoxy, propoxy and butoxy; alkyl = methyl, ethyl) have been synthesised. Their interaction with Nd^{3+} ion in the form of doped model has been discussed in terms of Slater-Condon, Landé and Judd-Ofelt parameters. The involvement of 4f-orbitals in the Nd^{3+} doped systems including deviation in symmetry has been discussed.

It has been well established that sulphur containing ligands have versatile pharmacological activity, which increases on complexation with metal ions[1]. Most important of them are sulphonanilide derivatives which have immense antibacterial activity. The complexing behaviour of lanthanide ions has not been studied extensively as compared to the transition metal ions. In continuation with our studies, we have undertaken the synthesis of sulphonanilides and an attempt has been made to characterize Nd^{3+} doped sulphonanilides on the basis of Judd-Ofelt, Slater-Condon and other theories. The complexing ability with respect to thermodynamic stability is poor in case of lanthanide complexes, so doped lanthanide ion in saturated solution of ligand has been undertaken as a system for electronic spectral study. The present work infers covalency in metal-ligand bonding in the systems undertaken. The study also provides some useful information regarding metal-ligand interaction and change in symmetry around lanthanide ion.

(A) Synthesis of Sulphonanilides: Sulphonanilides have been synthesised by the method reported in the literature[2, 3]. Structural formulae of synthesised sulphonanilides are as follows:



where

L	L_1	L_2	L_3	L_4	L_5	L_6
R^1	CH_3	C_2H_5	nC_3H_7	nC_4H_9	CH_3	C_2H_5
R^2	CH_3	CH_3	CH_3	CH_3	C_2H_5	C_2H_5

The IUPAC names of ligands are as follows:

L_1: 3-Carbomethoxy-4-hydroxy-N-methyl naphthalene-1-sulphonanilide.
L_2: 3-Carboethoxy-4-hydroxy-N-methyl naphthalene-1-sulphonanilide.
L_3: 3-Carbopropoxy-4-hydroxy-N-methyl naphthalene-1-sulphonanilide.
L_4: 3-Carbobutoxy-4-hydroxy-N-methyl naphthalene-1-sulphonanilide.
L_5: 3-Carbomethoxy-4-hydroxy-N-ethyl naphthalene-1-sulphonanilide.
L_6: 3-Carboethoxy-4-hydroxy-N-ethyl naphthalene-1-sulphonanilide.

(B) Preparation of Doped Systems: In the present work six systems of lanthanide ion doped in saturated solutions of these ligands have been prepared by adding 0.1 g. $NdCl_3 \cdot 6H_2O$ salt (supplied by Indian Rare Earth Ltd) per 10 mL of ligand solution. The solution spectrum of each system has been recorded in the range 350–950 nm by using standard spectrophotometer.

The values of various spectral parameters including oscillator strength, Energy, Slater-Condon, nephelauxetic ratio, Landé and bonding parameters etc. have been reported in Table-1. The observed changes in the various energy and intensity parameters show that the $f \leftrightarrow f$ transition resulting from spin-orbit interaction in Nd^{3+} ion is due to the interaction of f-orbital with the ligand present in the saturated solution. The calculation of various parameters involves Slater-Condon-Landé and Judd-Ofelt theories as reported by earlier workers[4–6]. Red-shift has been observed in all energy bands as compared to the free ion thereby establishing the validity of Slater-Condon-Landé theory. The r.m.s. deviation in energy varies from ±59.81 to ±103.07 in all the systems. The intensities of observed bands have been given in terms of oscillator strength (P), the r.m.s. deviation is very small varying from ±1.63 to 1.98 suggesting the validity of Judd-Ofelt theory for $f \leftrightarrow f$ transition. T_4/T_6 value varies from 0.98 to 1.97. It indicates variation in symmetry around doped Nd^{3+} ion in saturated ligand solution. The % rF_2 varies from 0.10 to 1.66 indicating decrease in interelectronic repulsion between metal and ligand. The values of nephelauxetic ratio (β) and bonding parameter ($b^{1/2}$) with little variation in it suggests that the 4f-orbitals are very slightly involved in the bonding in saturated solutions doped with Nd^{3+} ion. The % $r\zeta_{4f}$ varies from 4.00 to 6.95 indicating decrease in spin-orbit interaction in metal ligand bonding.

TABLE-1

VALUES OF VARIOUS PARAMETERS FOR Nd^{3+} DOPED SULPHONANILIDES

Ligand	T_4/T_6	F_2	F_4	F_6	ζ_{4f}	% $r\zeta_{4f}$	% rF_2	β	$b^{1/2}$	E^*_{exp}	$P_{exp} \times 10^{6*}$
L_1	1.97	330.84	51.25	5.35	844.22	4.50	0.10	0.9977	0.033	17241	21.6
L_2	0.98	326.52	52.64	5.29	848.61	4.00	1.40	0.9847	0.087	17182	17.6
L_3	1.44	327.41	52.88	5.32	833.36	5.73	1.13	0.9874	0.079	17182	30.2
L_4	1.45	325.66	54.35	5.19	822.56	6.95	1.66	0.9821	0.094	17241	18.6
L_5	1.52	330.20	51.32	5.32	844.52	4.47	0.29	0.9958	0.045	17241	30.0
L_6	1.38	326.80	52.80	5.29	847.26	4.16	1.32	0.9856	0.084	17196	22.5

*Values of hypersensitive peak $^4G_{5/2}$

Other parameters have also been computed so as to indicate variation in electronic spectral characterization.

ACKNOWLEDGEMENT

Authors are thankful to Dr. G.K. Joshi and Dr. H.K. Pandey of Dept. of Chemistry, Govt. Dungar College, Bikaner for their valuable suggestions and help.

REFERENCES

1. L. Bhal, J.P. Tandon and S.K. Sinha, *Curr. Sci.*, **55**, 566 (1984).
2. Vertkes Migradichian, Organic Synthesis, Vol. 2, Reinhold Publishing Corporation, New York, p. 1961 (1957).
3. S.S. Shrimali, N.D. Sharma, S. Kumar and B.C. Joshi, *Rev. Roum. Chim.*, **23**, 613 (1978).
4. B.K. Gupta, G.K. Joshi and P.R. Bhati, *Indian J. Pure and Appl. Phys.*, **28**, 525 (1990).
5. Neelam Naulakha, K.P. Soni and P.R. Bhati, *Asian J. Chem.*, **12**, 151 (2000).
6. M.P. Gotam, Ashok Yadav and S.N. Limaye, *Asian J. Chem.*, **10**, 415 (1998).

(*Received*: 2 January 2001; *Accepted*: 17 February 2001) AJC-2272