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NOTE

Variation in Symmetry Around Doped Nd^{3+} Ion in Saturated Solution of Sulphonanilides with Reference to Judd-Ofelt Electronic Spectral Parameter

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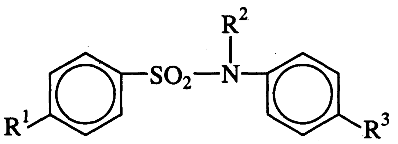
Three sulphonanilides have been synthesised. A comparative electronic-spectral characterization of Nd^{3+} doped sulphonanilide solutions has been done on the basis of Slater-Condon, Judd-Ofelt and Landé theories. The involvement of 4f-orbitals in Nd^{3+} doped systems including deviation in symmetry has been discussed.

Recently the studies on complexing behaviour of f-block elements with different ligands have been reported[1, 2]. In the present work sulphonanilides have been synthesised and an attempt has been made to characterize Nd^{3+} doped sulphonanilides on the basis of Judd-Ofelt, Slater-Condon and Landé theories.

Sulphonanilides have been synthesised by the method reported in the literature[3, 4]. Their structural formulas are as follows:



L	L_1	L_2	L_3
R^1	CH_3	C_2H_5	CH_3
R^2	H	CH_3	CH_3
R^3	CH_3	CH_3	OCH_3

L_1 : 4,4′-Dimethyl-N-ethyl benzene sulphonanilides.
L_2 : 4′-Methyl-N-methyl-3-nitrobenzene sulphonanilides.
L_3 : 4-Methyl-N-methyl-4′-methoxy benzene sulphonanilides.

To the saturated ligand solution 0.1 g $NdCl_3 \cdot 6H_2O$ salt (supplied by Indian Rare Earth Ltd.) per 10 mL was added and solution spectra were recorded in the range 350–950 nm by using standard spectrophotometer.

The calculated values of various spectral parameters have been reported in Table-1. Red shift has been observed in all energy bands as compared to the free ion thereby establishing the validity of Slater-Condon and Landé theory. Order of r.m.s. deviation in energy is $L_1 > L_3 > L_2$. The order of oscillator strength (P) for hypersensitive transition ($^4G_{5/2}$), *i.e.*, $L_3 > L_1 > L_2$ shows that maximum involvement of 4f-orbital in M—L bonding occurs in the case of L_3. Order of T_4/T_6 values, *i.e.*, $L_3 > L_1 > L_2$ indicates the variation in symmetry around doped Nd^{3+} ion in saturated ligand solution. Order of %rF_2 values, *i.e.*, $L_3 > L_1 > L_2$ shows that maximum decrease in inter-electronic repulsions between Nd^{3+} ion and ligand occurs when ligand is L_3. Order of % $r\zeta_{4f}$, *i.e.*, $L_1 > L_2 > L_3$ indicates that maximum decrease in spin-orbit interactions is observed with ligand L_3. Values of nephelauxetic ratio ($\beta < 1$) and bonding parameter ($b^{1/2}$) suggest covalency in the M—L bond in the present systems.

TABLE-1

Ligand	T_4/T_6	$P_{exp} \times 10^{6*}$	E^*_{exp}	r.m.s. dev in E	% $r\zeta_{4f}$	% rF_2	β	$b^{1/2}$
L_1	1.46	15.8	17182	±84.18	4.67	0.90	0.99	0.07
L_2	1.32	13.0	17241	±66.33	4.47	0.29	0.99	0.04
L_3	2.31	29.4	17211	±69.47	3.06	1.71	0.98	0.09

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