

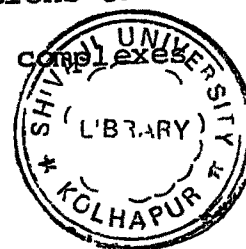
SYNOPSIS

Synopsis of the dissertation entitled "Studies of Some Charge Transfer Complexes" being submitted by Miss P.A. Muthane for the award of the degree of Master of Philosophy in Physical Chemistry.

The dissertation contains the results of the experimental work of four systems formed from two acceptors viz., 2,3-dichloro-1,4-naphthoquinone and 2,3-dichloro-5-nitro-1,4-naphthoquinone, and two donors viz., o-Ethylaniline and 2,6-dimethylaniline. The solvent was dichloromethane. The absorption spectra of these systems have been taken in the visible region at different temperatures.

The dissertation is divided into four chapters.

Chapter-I: This is an introductory chapter and contains the literature survey of charge transfer complexes. Brief account of the theory of charge transfer complexes is given. Mention has been made of the various methods employed for the determination of association constants and molar absorptivities. Optical method (i.e., UV-Visible spectroscopic method) is dealt in detail. Various equations such as Benesi-Hildebrand and its modifications by Scott, Scatchard and Rose-Drago have been explained. Equations for the evaluation of formation constants of 2:1 stoichiometric complexes are also given. Evaluations of free energies, enthalpies and entropies of formation of complexes



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have been explained. Similarly, equations for computations of oscillator strength and transition moment have been given.

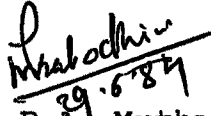
Chapter-II: This chapter deals with the experimental part of the work and preparation and purifications of chemicals used in the work. The instrument used is single beam UV-Visible Carlzeiss German make spectrophotometer. All chemicals are A.R. grade and are purified by standard methods and their physical constants compared well with literature values. The procedure for the synthesis of 2,3-dichloro-5-nitro-1,4-naphthoquinone is given. The visible absorption spectra of the acceptors are given.


Chapter-III: This chapter contains the experimental results and treatment of data. Typical absorption spectra in the visible region of all the four systems are given. For each system the acceptor concentration was kept constant whereas the donor concentration was varied. In all the cases, the donor concentration was much higher than the acceptor concentration. For each system 7-8 spectra were recorded. From peak optical densities of a particular system, the formation constants and molar absorptivities were computed by using Rose-Drago equation and the values have been tabulated. Thus the stoichiometry of the complexes was established. Using these values of equilibrium constants (formation constants) and molar absorptivities at different temperatures, the thermodynamic quantities such as free energies, ΔH and entropies have been calculated. For this purpose modified van't

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Hoff plots were used. Oscillator strengths and transition moments have been calculated from half band widths, molar absorptivities and peak frequencies using appropriate equations. All the values have been tabulated and necessary plots are given.

Chapter-IV: This is the discussion chapter. Effort has been made to explain the various properties of charge transfer complexes presented in Chapter-III. Variation in peak frequencies of charge transfer absorption bands of all the complexes studied are explained on the basis of electron affinity of the acceptors and electron donating ability of the donors. Stoichiometry of the complexes studied was established to be 2:1 (donor:acceptor). Linearity of Benesi-Hildebrand plots, not passing through origin, suggests the presence of 1:1 complexes in addition to 2:1 complexes in two systems viz., 2,3-dichloro-5-nitro-1,4-naphthoquinone acceptor complexes. Nearly temperature independency of molar absorptivities indicates the existence of single stoichiometric complexes. The negative values of the thermodynamic quantities such as change in free energies, enthalpies and entropies generally indicate the greater stability of complexes. The oscillator strengths and transition moments have been tabulated.


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