

PREFACE

Dielectric material plays an important role for its wide application in electronics and electrical technology. Scientists and research workers are mainly interested, on the other hand, in understanding the structure, shape and size of the dielectric molecules. In order to reveal the different aspects of dielectric materials the essential parameter like dipole moments, quadrupole moments, molecular polarisabilities, local fields etc. are needed to be determined. The present thesis is intended to throw much light on the structure, shape, size of a large number of nonspherical dielectric polar molecules dissolved in nonpolar solvents like C_6H_6 , CCl_4 , dioxane and n-heptane under high frequency electric field.

The other part of the thesis is concerned with the quantum mechanical approach to derive a formula of dipole moment of some isotopomer molecules like HD^+ , HT^+ etc. The molecules are interesting because the phenomenon of photodissociation occurs due to the interaction of such molecules with photons. Photodissociation is an important photon induced process. It is of great significance in the study of photochemical reactions, in modelling the ionised atmosphere and among others in determining the vibrational population of the molecular ions.

Under the action of the electric field the centre of gravity of positive and negative charges of a molecule is little displaced producing what is known as distortion polarisation. Due to existence of several polarisability factors the predicted dipole moment does not yield better result either in the static or in low frequency electric field. This difficulty was, however, removed altogether when the static electric field is replaced by an alternating electric field of frequency in the order of $10^6 \sim 10^9$ Hz. As a result all the polarisability factors other than orientational polarisation are thus eliminated.

On account of inertial effect of polarisation the molecule does not rotate immediately with the rapid reversal of the electric field, but undergoes a delay or lag in response for a certain time. When the external field is removed all types of polarisation decay exponentially with time. The time in which the polarisation is reduced to $1/e$ times its original value is called the relaxation time and is usually denoted by τ . The polar mol-

ecules in nonpolar solvents usually absorb energy much more strongly in the high frequency electric field of 10 GHz. Analysing the high frequency absorption relaxation data for radio and microwave regions one can easily get the relaxation time with the help of available Debye and Smyth model. This relaxation time τ is due to the molecular rotation as a whole. There is also a probability of rotation of a part of the molecule under the hf electric field. So the possible existence of multiple relaxation phenomena was proposed by Budo (1938). Bergmann et al (1960), however, considered that the polar molecules are supposed to possess two relaxation times τ_2 and τ_1 , one due to whole molecular rotation (τ_2) and other, due to rotation of a part of the molecule called intramolecular relaxation time (τ_1). They used Cole - Cole (1941) plot to arrive at the desired value. Bhattacharyya et al (1970), subsequently simplified the above procedure to get two relaxation times τ_2 and τ_1 of a pure polar solute from the dielectric relaxation parameters measured at least at two different frequencies of the applied electric field. We, under such context, have been able to predict double relaxation phenomena of polar solutes in a nonpolar solvent from the values of the dielectric relaxation parameters measured under a single frequency electric field. In the Part A of the present thesis several chapters deal with the existence of double or mono-relaxation times.

Chapter III is concerned with nonspherical polar molecules like disubstituted benzenes and anilines in nonpolar solvents like C_6H_6 or CCl_4 under 9.945 GHz electric field.

Chapter IV deals with the prediction of double or single relaxation time at 22.06, 3.86 and 2.02 GHz electric field for three isomers of anisidines and toluidines.

In chapter V an attempt has been made to show that isomers of anisidines and toluidines show two relaxation times at 9.945 GHz electric field which seems to be the most effective dispersive region for such polar molecules.

In chapters VI and VII the long chain alcohols are studied at 24.33, 9.25 and 3.00 GHz electric fields only to show the fact that they always show double relaxation times at each frequency of electric field.

In chapter VIII binary aprotic polar mixtures like N, N-dimethyl formamide and dimethyl sulphoxide (DMF + DMSO) as well as single aprotic liquid DMSO and N,N

diethyl formamide (DEF) in C_6H_6 and CCl_4 are studied at 3 cm. wavelength electric field to show the different associational aspects in them.

Chapter IX deals with the experimental works performed at IACS Laboratory to show the possible occurrence of double relaxation times for the aprotic liquids like dimethyl sulphoxide (DMSO), N, N-dimethyl acetamide (DMA), N,N-dimethyl formamide (DMF), N, N-diethyl formamide (DEF), N-methyl acetamide (NMA) etc. dissolved in C_6H_6 at different temperatures. To know the actual fact measurements on ϵ'_{ij} , ϵ''_{ij} , ϵ_{oij} and $\epsilon_{\infty ij}$ of them were accurately performed.

Part B of the, thesis is presented in one chapter X. It consists of estimation of dipole moments of HD^+ , HT^+ etc. molecules from quantum mechanical point of view using Morse potential.

Thus the first part of the thesis beautifully explains the double relaxation phenomenon of nonspherical polar molecules in nonpolar solvents under hf electric field, in a very simple and straightforward way for the first time. It, therefore, minimizes the experimental hazards in determining dielectric relaxation parameters at more than one frequency of the electric field. From this point of view the proposed method is thought to be superior one in comparison to other existing methods.

The part B of the thesis being the last part is included in chapter X. It appears to reveal that isotopomer molecules like HD^+ , HT^+ etc. are expected to obey Morse potential (1929) to yield the dipole moment μ as estimated by Saha (1974) indicating the fact that the molecules obey Morse potential.

A conclusive part is also added in the last Chapter XI of the thesis only to get a brief summary of the entire works presented in the thesis.

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