

Dielectric relaxation behaviour of glycine in aqueous solution medium in the microwave frequency region

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Received 6 December 2006; accepted 28 February 2008

A study on the dielectric properties of glycine in aqueous solution medium in the microwave frequency region (130 MHz-20 GHz) is carried out using the open-ended coaxial probe technique. Dielectric parameters such as dielectric constant, dielectric loss of various weight percentage levels of glycine in double distilled aqueous medium such as water are determined. It is observed that the real part of dielectric permittivity decreases and imaginary part of the dielectric permittivity increases with increase in the weight percentage level of glycine in water. From these parameters we calculated the relaxation time and its behaviour is analysed. Dipole moment value is calculated from the optimized geometrical structure of the glycine molecule from the AM₁, PM₃, and MNDO *ab initio* quantum mechanical calculations using the Argus Lab chemical modeling Software 2004.

Keywords: Complex permittivity, Relaxation time, Dipole moment

The interaction of electrical energy with matter is determined by the electromagnetic properties of the material. On a macroscopic scale under steady state conditions, these properties are conventionally described by the permeability and the permittivity of a material. Increasing use of microwaves and millimeter waves in such diverse fields as communications, radar, medicine, biology, agriculture and industrial process demands accurate data on dielectric properties of materials. The characterization of dielectric materials includes the measurement of complex permittivity as a function of frequency at a given temperature or as a function of temperature at a given frequency. The measurement of dielectric properties at wide frequency range gives the information regarding the frequency conduction mechanism, interfacial polarization, molecular dynamics and relaxation behaviour phenomena¹.

Aqueous studies of amino acids at different concentration levels were carried out for determining the nature of interaction exist between the molecules due to hydrogen bonding, dipole moment and the relaxation behaviour phenomena. The functional groups present in the amino acid are alcoholic, ketone, and amine group respectively. The nature of interaction that exists between the $-C=O$, $-OH$ and

$-NH$ groups in a polar medium such as water plays an important role in the biological systems and drug synthesis.

Recently open-ended coaxial lines have attracted many researchers for their application in non-destructive measurements of the complex permittivity of materials. These techniques are very attractive, particularly for in vivo measurements of biological materials²⁻⁴. Open-circuited air-filled coaxial lines are also used as calibration standards for microwave measurements. For non-destructive measurement of permittivity, the sample material terminates the open end of coaxial line, and the input reflection coefficient of the system is measured at a desired frequency and temperature. These data can be related to the complex permittivity of the material, and this data can be analysed by using Misra-Blackham model⁵ and coaxial probe model^{6,7} (lumped parameter model).

In this paper, we measured the complex permittivity of glycine in a different weight percentage levels (0.1-1 g) in a aqueous medium by using the open-ended coaxial probe method and dipole moment of the glycine molecule is calculated from the Hamiltonian theoretical quantum mechanical calculations such as AM₁, PM₃ and MNDO by using the Argus lab chemical modeling software 2004. The average relaxation time is calculated from the respective Debye plots⁸.

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Experimental Procedure

One of the amino acid glycine is taken in a different weight percentage levels (0.1-1 g) and diluted in a double distilled water. The complex dielectric permittivity of different weight percentage levels of glycine in a aqueous medium is measured in the microwave frequency range (130 MHz-20 GHz) by using the open-ended coaxial probe method and concern data of these systems is analyzed by using the coaxial probe model (lumped parameter model). The refractive index ($\epsilon_\infty = \eta^2$) of the above system is determined using the Carl-zeiss Abbe refracto-meter with sodium D light as a source.

Results and Discussion

Variation of real and imaginary part of the dielectric permittivity of different weight percentage levels of glycine in aqueous solution medium are shown in Fig. 1 and error in the measurement of real part of dielectric permittivity is 3% and imaginary part of dielectric permittivity is 4%. By plotting the graph between real and imaginary part of dielectric

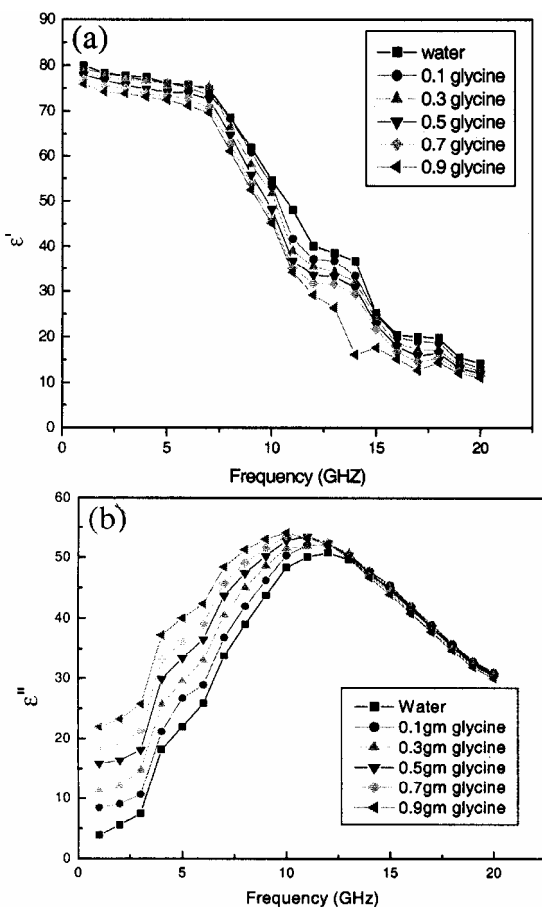


Fig. 1—Variation of real and imaginary part of dielectric permittivity with respective frequency

permittivity we obtain Debye behaviour for different weight percentage levels of glycine in aqueous solution medium. The average relaxation time is calculated from the debye plot and dipole moment value is calculated from the theoretical Hamiltonian quantum mechanical calculations such as AM1, PM3 and MNDO by using the Argus lab and which are given in Table 1. The calculation of the dipole moment of the glycine molecule is not possible by experimental methods due to dissolving nature of amino acids in a non polar solvent medium.

From the Fig. 1a it is observed that the real part of the dielectric permittivity values decreases with increase in frequency and also from the Fig. 1b it is observed that there is a strong absorption peak at 12 GHz and decreasing with increase in frequency. Due to the formation of hydrogen bonding between glycine and aqueous medium such as water there is a change in the intensity level of absorption. As a weight percentage level of a glycine in an aqueous medium increases there is an increase in the number of hydrogen bond network. The increase in the hydrogen bond network causes the decrease in the real part of dielectric permittivity and increase in the imaginary part of dielectric permittivity compared to water.

The increase in the number of hydrogen bonds in the aqueous medium causes the increase in the relaxation time values and which is shown in Fig. 2.

Table 1—Dipole moment values from the theoretical Hamiltonian quantum mechanical calculation

Sample	AM1	PM3	MNDO
Glycine	4.546	4.397	4.389

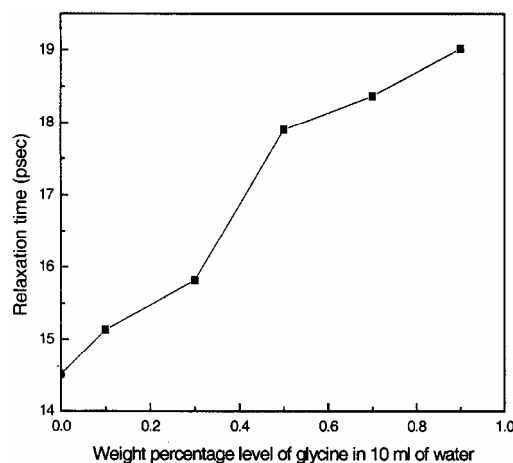


Fig. 2—Variation of relaxation time with respective weight percentage level of glycine in 10 mL of water

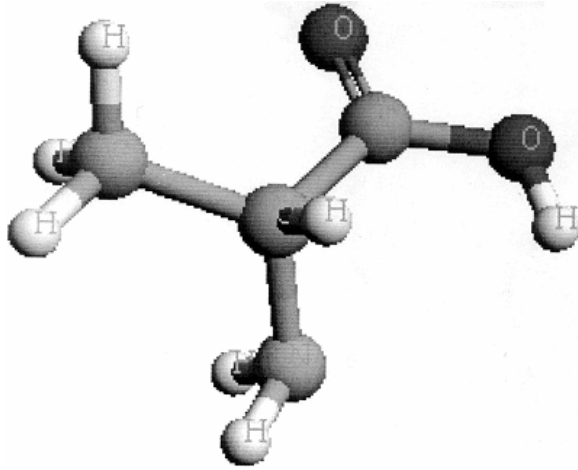


Fig. 3—Optimized geometrical structure from the AM1 Hamiltonian quantum mechanical calculations

As weight percentage of glycine increases in an aqueous medium there is an increase in the number of self-associated groups formed by the hydrogen bonds. These self-associated groups are responsible for increase in the imaginary part of dielectric permittivity due to this relaxation time values increase with increase in weight percentage of glycine.

Dipole moment value is calculated from the optimized geometrical structure of the glycine, molecule in an aqueous medium from the AM₁, PM₃, and MNDO quantum mechanical calculations using the Argus Lab chemical modeling Software 2004 and

the values that are given in Table 1 and the structure is shown in Fig. 3.

Conclusions

The real part of dielectric permittivity decreases and imaginary part of dielectric permittivity and relaxation time values increase with increase in weight percentage level of glycine in an aqueous solution medium. The increase in relaxation time values may be due to the formation of self-associated hydrogen bond groups by glycine molecule in an aqueous solution medium

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