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High Frequency Acoustic Absorption in Acetates and Formates using Artificial Neural Network

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ABSTRACT
Artificial neural network (ANN) is applied to methyl and ethyl acetate as well as methyl, ethyl, propyl and butyl formate respectively to study ultrasonic absorption due to rotational isomers at different temperatures and frequencies. From statistical analysis, the results predicted through neural network have been found to be accurate. Further, the trained weights obtained through the trained network are used to predict the ultrasonic absorption at different frequencies and temperatures**.**
Keywords - ANN, acetate, formate, Frequency, Temperature.

I. INTRODUCTION

When high frequency sound waves are passed through the liquid there are structural changes and consequently molecules go to higher energy levels. After the passage of sound waves these molecules return comes to ground energy levels and relaxation takes place. Here the molecules vibrate, rotate and transmit energy. Stokes recognized the possibility of volume viscosity in liquids [1]:

$$\left(\frac{\alpha}{f^2}\right)_{(obs)} = \frac{2\pi^2}{\rho c^3}\left[\frac{4\eta_s}{3} + \eta_v\right] \quad (1)$$

The contribution [2] arising from shear viscosity (η_s) is,

$$\alpha_1 = \frac{8\pi^2}{\rho c^3}\eta_s f^2 \quad (2)$$

And due to thermal conductivity K is,

$$\alpha_2 = \frac{2\pi^2}{\rho c^3 c_p}(\gamma - 1)Kf^2 \quad (3)$$

Where ρ is the density of the liquid, C_P is the specific heat per unit mass at constant pressure, K is thermal conductivity, γ is the ratio of specific heats and c is ultrasonic velocity. The absorption in excess which is caused due to additive effects of shear viscosity and thermal conductivity is known as classical absorption.

$$\alpha_{classical} = \alpha_1 + \alpha_2$$

$$(\alpha/f^2)_{classical} = \frac{2\Pi^2}{\rho c^3}\left\{\frac{4\eta_s}{3} + \frac{K(\gamma-1)}{C_p}\right\} \quad (5)$$

The difference between the measured absorption coefficients and the classical absorption is referred to as excess absorption.

$$\alpha_{Excess} = \alpha - \alpha_{classical}$$

$$\frac{2\Pi^2\eta_v f^2}{\rho c^3} \quad (6)$$

The excess absorption is caused due to structural changes as well as due to rotational isomers. Structural relaxation in acetates and formates is caused due to rotational isomers. Karpovich [3] attributed the relaxation processes caused due to disturbance by the sound wave at the equilibrium between rotational isomers in many organic liquids. Slie and Litovitz [4] studied the effect of pressure and temperature on rotational isomeric relaxation in ethyl acetate. Formates are studied by various researchers [1-9] and these systems are characterized by the C-O bond. In case of methyl, ethyl, propyl and butyl formate the possibility of two rotational isomers *cis* and *trans* is formed. The rotational isomers *cis* refers to the C-O bond on either side of the structure whereas *trans* refers to C-O bond on the opposite side of the structure.

Recently Mirzaev *et al* [10] made experimental study in butyl formate and observed that the ratio of rotational isomers varies with temperature. The experimental complexities involved in determination of absorption and lack of availability of data associated with the frequency and temperature dependence of the absorption in the literature [3-11] lead the present work to formulate the objective of generation of absorption data using Artificial Neural Network. For statistical analysis, we have used RMS (root-mean-squared) error, absolute fraction of variance (R^2) [12] and coefficient of variation (cov) [13].

II. ARTIFICIAL NEURAL NETWORK

Nature has gifted human beings with the power to think and apply it to various processes. The power of human brain is reflected through the functioning of neurons. The neuron consists of dendrites, soma, axon and synapse. Dendrites receive signals and pass it on to the soma, and axon transmits signals which are to be sent to other neurons through synapses. Motivated by the functioning of neurons, scientists have applied this concept to the complex problems [12-19] which are difficult to solve using traditional methods. They specified this neuron as 'artificial neuron'. The artificial neuron accepts any number of inputs simultaneously. Using weights these inputs are connected to processing element, where the summation of these weighted inputs is taken. With the help of transfer functions these are processed and converted into the output. The term Artificial Neural Network was inspired by the functioning of biological neural processing. A neuron is a fundamental processing unit of information. These neurons are interconnected to units in ANN. Artificial neurons act as building blocks in Artificial Neural Network (ANN). Each unit consists of input output characteristics and makes use of a local computing or function. The nature of output depends upon its input - output characteristics, its interconnection to other units, and external input. The hidden layer of feedforward network consist of logsig transfer functions. It is a continuous and differentiable transfer function. The range of logsig is $(0,+\infty)$. It takes the form,

$$F(Z) = \frac{1}{1 + \exp(-Z)}$$

where Z is the weighted sum of the inputs.

III. TRAINING PROCEDURE

Inspired by the working efficiency of artificial neurons, we have developed a model for the prediction of ultrasonic absorption in formats and acetates. ANN requires sufficiently large data to form the relationship between input and output pairs. The required experimental data for training the network for formates and acetates is taken from the literature [11]. The models are trained using the Leverberg – Marquardt learning algorithm [20] and calculates the output vector for each input vector. The hidden layer of the network for formates consists of 5 logsig transfer functions and the output layer consists of 1 purelin transfer function. For methyl acetate it consists of 6 logsig transfer functions and the output layer consists of 1 purelin transfer function and for ethyl acetate it consists of 9 logsig in the hidden layer and 1 purelin transfer function in the output layer. The outputs of hidden and output neurons evaluated an error term by comparing the calculated output vector and the actual output vector called target. Using this error term, the weights and biases are updated to decrease the error. This procedure was repeated until the error goal of $1x10^{-10}$ and 2000 epochs are reached. The sum squared error was used as the performance function and works out to be 0.000718341, 0.000526597, 0.00669705 and 0.0135166 for methyl, ethyl, propyl and butyl formate. The mean squared error was used as the performance function and works out to be 0.000227214 for methyl acetate and for ethyl acetate, it is found to be 0.335076.

IV. RESULTS AND DISCUSSIONS

S. No	Sample	F (MHz)	R^2	RMS	COV
1	methyl formate	15 30	0.999 0.993	2.9211 3.0427	3.925 8.967
2	ethyl formate	15 18	0.999 0.997	3.8651 3.7338	6.971 7.007
3	propyl formate	17.9	0.999	8.2287	7.725
4	butyl formate	14.6 22.5	0.999 0.999	2.4661 7.7552	2.418 8.953

5	methyl acetate	9.76 11.85 14.6	0.998 0.984 0.982	10.825 13.566 12.045	12.82 17.07 16.46
6	ethyl acetate	4.7	0.999	8.0119	5.126

Statistical analysis is as shown in the TABLE .

During testing phase of the ANN model, once the model is trained the experimental values of temperatures and frequencies are provided to it which the network has not seen earlier. To study the effect of temperature on the various parameters, the trained weights and biases are used which were stored in the file. Statistical analysis shows that ANN is successful in predicting the values of absorption at various frequencies and temperatures. In our application, temperature values are normalized as $t = T / 1000$, whereas frequency values are normalized as $f = F / 100$. With the help of trained weights biases we have predicted values of absorption at different temperatures and frequencies on which absorption data is not available and studied that. We can provide the data if anyone is interested.

The relaxation absorption in formate is caused due to rotational isomers. It is observed that in methyl formate at lower frequencies, absorption shows higher variation than at the higher frequencies. There is rapid growth of absorption with temperature. The ratio of rotational isomers at higher energy levels increases with increase in temperature. At higher frequencies, absorption remains almost constant with temperature. The reason may be that at higher frequencies, the higher energy levels are completely occupied with rotational isomers and there is no breaking of hydrogen bonds. In ethyl formate, the variations in absorption takes place on higher temperatures at lower frequencies. According to Tabuchi [5], the molecule of ethyl formate has resonance structure hence there exists two stable isomers of planar having resonance energy. The ratio of rotational isomers increases with increase in temperature. Also, the two states consist of rotational isomers. The isomers increase with increase in temperature on the higher energy state. On higher temperatures and at lower frequencies the breaking of hydrogen bonds takes place due to rotation of isomers and absorption increases. In propyl formate there is almost no difference between absorption values at higher frequencies with increase in temperature. At lower frequencies, the behavior of proply formate molecules is different from other formates. According to Piercy *et al.* [7] the influence of the medium also contributes to the difference in energy of the isomers. At higher temperatures, the energy levels are completely occupied with the rotational isomers and isomers find no space to rotate. With rapid increase in temperature there is no energy transfer between the energy levels and the absorption of the molecules remains almost constant. Moreover, in butyl formate at lower temperatures, the isomers jump to higher energy levels. The energy exchange takes place and the absorption increases. The breaking of hydrogen bonds occurs more in butyl formate as it has highest molecular weight as compared to other formates. Further it is observed that at 1 MHz, the variation of absorption is more as compared to 10 MHz and 30 MHz in methyl acetate. According to Karpovich [3], the hydrogen bonds break and the molecules go to the excited state and absorption increases. At higher temperature hydrogen bond break and hence absorption increases. At higher frequencies, the energy levels are occupied more energy is required to break the hydrogen bond the variation is less at 10 and 30 MHz. In case of ethyl acetate, the variation of absorption is completely different as compared with methyl acetate. According to Karpovich [3], the relaxation frequency at 293 K is 11.4 MHz. The change in absorption is less at lower temperatures as compared to higher temperature. At lower temperature the hydrogen bonds break and absorption increases. As the temperature increases, the cluster formation slows down and absorption decreases. With increasing temperature the hydrogen bonds start breaking and absorption increases.

V. CONCLUSIONS AND FUTURE

In the present study, the ultrasonic absorption in formates and acetates are studied at various frequencies and temperatures. The R^2 value is found to be 0.9999 which indicates the accuracy of ANN. The variation in absorption takes place at lower frequencies as compared to higher frequencies in all formates under study. The absorption is found to be more for higher formates at lower frequencies. In methyl acetate, the variation of absorption is found to be more at higher temperature for lower frequencies, whereas in case of ethyl acetate at lower temperature the variation of absorption is more as compared to at higher temperature. ANN is found to be suitable tool for the prediction of ultrasonic absorption at various temperatures and frequencies in formates and acetates.

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