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# Intermolecular Interaction of Methyl Formate with 1-butanol, 1-pentanol and 1-hexanol at 303K

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**Abstract**

Intermolecular interaction among methyl formate with selected primary alcohols studied using Time Domain reflectometry at 303K. Dielectric constants, dielectric loss, were determined. The parameters changed with concentration and chain length of alcohols in methyl formate system. Strength of intermolecular interaction of alcohols with methyl formate determined as 1-butanol<1-pentanol<1-hexanol.

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## Introduction

Intermolecular interaction among the liquid mixtures takes place a vital role in chemical industries and reseaech field.[1-3] The dielectric relaxation studies take a vital role to elucidate the nature of interactions in a liquid system with polar and non polar molecules.[4,5] Methyl formate is used in various chemical and pharmaceutical industries.

Alcohols are highly polar and self associated through hydrogen bonding. The carbonyl group (C=O) exist in the methyl formate tends to form hydrogen bonding with hydroxyl (OH-) group of selected alcohols. The present work is an attempt to elucidate the molecular interactions between of methyl formate with1-butanol, 1-pentanol and1-hexanol using time domain reflectometry technique at 303K.

## Materials and Methods

Methyl formate and alcohols of AR grade were obtained from E-Merck India and used with out further purification. The purity of liquids analysed with the standard physical quality values. Dielectric constant (ε' ) and dielectric loss (ε" ) were obtained using oscillator of frequency 9.36 GHz at 303K. Abbe's refractometer was used to determine refractive indices (μ) of the binary liquid system. Viscosities of the liquid mixture were measured by Ostwald's viscometer. Densities were measured by using 5cc specific gravity bottle.

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## Methods

### Higasi's Method

Dielectric relaxation time (τ) was determined using Higasi's method[6]. Considering $\epsilon_0$ ϵ ,'ε" , $\epsilon_\infty$ linearly change with concentration of solute. The slopes $a_0$,a',a"and $a_\infty$ were determined by the experimental results. Here

$$\varepsilon_0 = \varepsilon_1 + a_0 w_2$$

$$\varepsilon' = \varepsilon_1 + a' w_2$$

$$\varepsilon'' = a'' w_2$$

$$\varepsilon_\infty = \varepsilon_{1\infty} + a_\infty w_2 \quad \text{.....(1)}$$

$$\tau_{(1)} = \frac{a''}{\omega(a' - a_\infty)}$$

$$\tau_{(2)} = \frac{(a_0 - a')}{\omega a''}$$

$$\tau_{(0)} = \sqrt{\tau_{(1)}\tau_{(2)}} \quad \text{.....(2)}$$

Mean relaxation time($\tau_0$), dielectric relaxation $\Delta F_\tau$ and viscous flow were determined by Eyring's equation[7]

$$\tau = \left(\frac{h}{kT}\right)\exp\left(\frac{\Delta F_\tau}{RT}\right) \quad \text{.....(3)}$$

$$\eta = \left(\frac{Nh}{V}\right)\exp\left(\frac{\Delta F_\eta}{RT}\right) \quad \text{.....(4)}$$

### Cole-Cole Method

Determined values of ε0, ε,' ε" and ε∞ are fitted in a graph. Diameter angle with respect to centre from ε∞ point and abscissa axis is equal to ϖα/2. Relaxation time τ was determined by

$$(\omega\tau)^{1-\alpha} = V/U \quad \text{.....(5)}$$

**Table 1-Dielectric constant ($\varepsilon_0$), relaxation time (τ) of methylformate with alcohols at 303K**

| Volume % of alcohols | $\varepsilon_0$ | ε' | ε" | $\varepsilon_\infty$ | Relaxation Time τ (ps) | | | | Activation energy | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Higasi's | | | Cole-Cole | | |
| | | | | | $\tau_{(1)}$ | $\tau_{(2)}$ | $\tau_{(0)}$ | τ | $\Delta F_\tau$ kJ/mol | $\Delta F_\eta$ kJ/mol |
| **System : Methylformate + 1-Butanol** | | | | | | | | | | |
| 0 | 3.38 | 2.7382 | 0.9513 | 2.3334 | 9.957 | 12.834 | 11.28 | 4.5509 | 7.213 | 3.38 |
| 25 | 3.2946 | 2.7627 | 0.966 | 2.3306 | 10.37 | 13.212 | 11.714 | 4.9086 | 7.514 | 3.2946 |
| 50 | 3.2204 | 2.7669 | 0.9863 | 2.3453 | 11.637 | 13.73 | 12.645 | 6.9302 | 7.871 | 3.2204 |
| 75 | 3.1217 | 2.7515 | 0.9765 | 2.3376 | 10.132 | 13.786 | 11.833 | 7.6757 | 7.577 | 3.1217 |
| 100 | 3.0594 | 2.734 | 0.9688 | 2.3264 | 9.845 | 12.708 | 11.196 | 8.0992 | 7.143 | 3.0594 |
| **System : Methylformate + 1-Pentanol** | | | | | | | | | | |
| 0 | 3.2582 | 2.6675 | 1.624 | 2.9277 | 11.875 | 17.111 | 14.297 | 16.1191 | 7.465 | 3.2582 |
| 25 | 3.1609 | 2.6661 | 0.9114 | 2.8304 | 10.594 | 13.94 | 12.162 | 11.4032 | 7.297 | 3.1609 |
| 50 | 3.1595 | 2.6654 | 0.9121 | 2.8304 | 10.307 | 15.256 | 12.561 | 16.8527 | 5.974 | 3.1595 |
| 75 | 3.0846 | 2.6514 | 0.903 | 2.7548 | 9.88 | 11.777 | 10.79 | 10.8985 | 6.835 | 3.0846 |
| 100 | 3.0832 | 2.6577 | 0.9044 | 2.7527 | 9.866 | 12.519 | 11.119 | 17.6591 | 7.045 | 3.0832 |
| **System : Methylformate + 1-Hexanol** | | | | | | | | | | |
| 0 | 3.2428 | 2.6892 | 0.931 | 2.3488 | 12.932 | 20.107 | 16.152 | 18.9415 | 7.36 | 3.2428 |
| 25 | 3.1343 | 2.6717 | 0.9114 | 2.3425 | 11.854 | 16.866 | 14.15 | 14.9606 | 7.143 | 3.1343 |
| 50 | 3.1098 | 2.6724 | 0.9086 | 2.3446 | 11.959 | 16.747 | 14.164 | 19.7304 | 7.304 | 3.1098 |
| 75 | 3.0923 | 2.6675 | 0.9051 | 2.3369 | 11.063 | 14.045 | 12.47 | 14.6169 | 6.667 | 3.0923 |
| 100 | 3.0335 | 2.6241 | 0.9009 | 2.3362 | 11.014 | 13.24 | 12.078 | 20.5235 | 6.912 | 3.0335 |

**Result and Discussion**

Dielectric parameters of the liquid mixtures have been determined as shown in the Table-1. The relaxation time varies with nature of bonding present in the liquid system.

In this study, relaxation time ($\tau$) changed with concentration and carbon chain length of alcohols. It shows that formation of hydrogen bond in carbonyl group of methyl formate and hydroxyl group of the alcohols. More over the $\varepsilon 0$ value changed with concentration of the alcohols. It reveals that decrease in the molar volume of the rotated molecules reduces the number of dipoles in the liquid mixture. It signifies that molar free energy of activation for viscous flow ($\Delta F_{\eta}$) is greater than dielectric relaxation ($\Delta F_{\tau}$). It may elucidates that viscous flow involved in rotational and translation vibration of molecules [8-10]. Hence strength of molecular interaction changed with proton donating ability of alcohols which was in the order of l-Butanol<1-Pentanol<1-Hexanol.

**Conclusion**

Dielectric relaxation parameters have been determined for methyl formate with 1-Butanol,1-Pentanol and 1-Hexanol prepared with various concentrations at 303K. Relaxation time changed with increasing proton donor in the liquid systems. The deviation of dielectric parameters with alcohols signifies that strength of molecular interaction of alcohols with methyl formate was in the order of 1-Butanol<1-Pentanol<1-Hexanol.

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**Conflict of interest**

There is no conflict of interest between the authors.

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