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Investigation on CI Engine Performance Through Molecular Structure Determination of Multifunctional Fuel Additives

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Abstract— Multi-functional fuel additives containing oxidation prevention agents and oxygenates.. It can be offered to improve the combustion efficiency, reduce emissions and carbon footprint. Amine act as a oxidation prevention agents and alcohol can be used as oxygenates. They are utilized to diminish the exhaust emissions when burning fuel. Therefore it is appeared vital to look at the molecular interaction considers on those added substances. In this paper the structure of amine and alcohol mixtures such as 1-butanol in (benzene + Ethylenediamine) and 1-propanol in (benzene +Ethylenediamine) can be investigated by dielectric relaxation method through the dielectric parameters such as static permittivity (ε_0), Permittivity at optical frequency (ε_∞), dielectric constant at microwave frequency (ε'),dielectric loss (ε'') at microwave frequency, density (ρ) and the coefficient of viscosity (η)at three different temperatures 303K, 313K and 323K are reported and in those mixtures, complex formation through hetero interaction identified and its combustion properties discussed.

Index Terms— dielectric loss, multifunctional fuel additive, oxygenates, relaxation time

I. INTRODUCTION

Fuel of substandard quality has the tendency to wear components, cause stickiness in valves and clog the filters. Additives and diesel fuel enhancement products were developed to resolve such issues. Here are 7 ways in which diesel fuel additives help engines: They –Upgrade and stabilize fuel by minimizing the amount of sludge and fuel tank contaminants, Cleanse and protect the fuel system components, eliminate varnish and other deposits from fuel tank to prevent plugging, Enhance power and diesel fuel economy, Protect the engine against low sulfur fuels to reduce wear, help to eliminate water from fuel, Offer hot and cold weather protection to the diesel engine. Multifunctional diesel additive packages are frequently more complex and may combine cetane number improver, Oxygenates, antifoam additive, corrosion inhibitor, antioxidants, metal deactivators and demulsifier [1].The oxygenate additives contain oxygen in their chemical structure. These compounds increase the oxygen content of the fuel and optimize the combustion process. They reduce soot and carbon monoxide produced by combustion of fuel. The common oxygenates are divided into two subgroups alcohols and ethers [2]. Literature survey shows that Butanol is a feasible alternative to ethanol due to its higher energy density, being less prone to water contamination, less corrosive, better blending stability and higher cetane number with respect to ethanol [3]. Ethylenediamine inhibit oxidation and provide stability in fuel burning. They prevent decomposition of lubricant. The present work was aimed to get better understanding of the nature of molecular interaction based on the study of the temperature dependent dielectric relaxation in multifunctional fuel additive mixtures of 1) 1-butanol in (benzene +Ethylenediamine) and 2) 1-Propanol in (benzene + Ethylenediamine) at microwave frequencies.

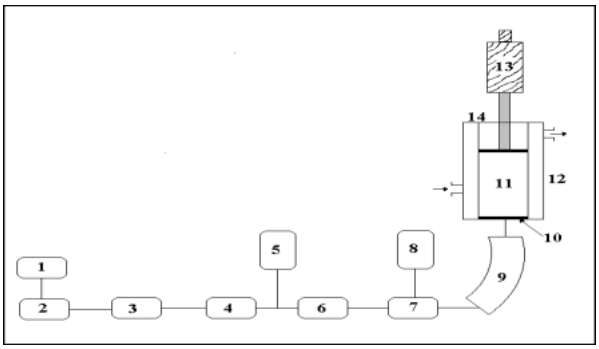
II. MATERIALS AND METHODS

Alcohol and amine used in the present study were of AR grade and were all procured from SRL, India. The static permittivity ε_o at 1 KHz was measured using a digital VLCR-7 meter supplied by M/S Vasavi electronics, India, after calibrating it for standard liquids like carbon

ISSN:0971-1260

Vol-22-Issue-10-November-2019

tetrachloride, benzene, toluene and chlorobenzene. The permittivity at optical frequency ε_∞ was obtained by squaring the refractive Index for sodium D-line, which was measured with the help of an Abbe's refractometer. The uncertainties in static permittivity, refractive index and density were ±0.0005, ±0.0002 and ±0.0001 g/cc respectively. All measurements were made at 303±1K, 313±1K, and 323±1K using a water circulating thermostat arrangement. For density measurement, a 10ml specific gravity bottle was employed. Its volume at the given temperature was determined using pure water. Density measurements of each sample were made at the required the losses due to evaporation of the sample were minimized. The viscosities of the mixtures were measured by using Ostwald's viscometer. ε' and ε" were measured by using a standard liquid cell supplied by M/s. SISCO Ltd., Allahabad, in conjunction with a X- band microwave set up, at 9.75GHz and temperature 303K,313K and 323K respectively. It is shown in fig 1.The constant



temperature was maintained by water – circulating thermostat supplied by Ragga Industries, Chennai, India. The fluctuation in temperature was ± 0.1K.

Fig 1.Microwave X – Band Test Bench

1.Power supply 2.Reflex Klystron K – 27 3.Tuner 4.Ferrite isolator 5.Frequency meter 6.Attenuator 7.Slotted line carriage 8.Crystal detector 9. H-Plane bend 10.Teflon window 11.Liquid cell 12.Constant temperature jacket13.Micrometer head 14.Plunger

III. THEORY

The dielectric relaxation time (τ) was calculated using Higasi's method [4-8]. Assuming ε_0, ε' , ε" and ε_∞ vary linearly with weight fraction w_2 of the solute. We have:

$$\varepsilon_0 = \varepsilon_1 + w_2 a_0 \quad ; \quad \varepsilon' = \varepsilon_1 + w_2 a' \; ;$$

$$\varepsilon'' = a'' w_2 : \varepsilon_\infty = \varepsilon_{1\infty} + a_\infty w_2 ; \quad \varepsilon_\infty = \varepsilon_{1\infty} + a_\infty w_2$$

The following expression were used for obtaining ε' and ε"

$$\varepsilon' = \left(\frac{\lambda_0}{\lambda_c}\right)^2 + \left(\frac{\lambda_0}{\lambda_d}\right)^2$$

$$\varepsilon'' = 2/\pi \left(\frac{\lambda_g \lambda_0^2}{\lambda_d^3}\right)\left(\frac{d\rho}{dn}\right)$$

Where λ_d is the wavelength in the dielectric medium, λ_g , the wave guide wavelength, λ_0, the free space wave length, λ_d, the cut off wavelength and $1/\rho$ is the standing wave ratio obtained by using a short circuited movable plunger. The uncertainties in the measurement of ε' and ε" are 1% and 5% respectively. The relaxation time for various solutions was also obtained in term of two Debye relaxation mechanisms with the help of the following equation for dilute solution of weight fraction w_2

$$\tau_1 = \frac{a''}{\omega (a' - a_\infty)} \qquad \tau_2 = \frac{a_0 - a'}{\omega a''}$$

Where τ_1 is a sort of intramolecular relaxation time , τ_2 is dielectric relaxation time for overall rotation of the whole molecule , τ_o is the most probable relaxation time, ω is the angular frequency, τ_1 and τ_2 depending on both the weight factor of such mechanism at a given concentration and temperature.

$$\tau_0 = \frac{1}{\omega}\left(\frac{A^2 + B^2}{C^2}\right)^{\frac{1}{2(1-\alpha)}}$$

where

$$A = a''(a_0 - a_\infty)$$

$$B = (a_0 - a')(a' - a_\infty) - a''^2$$

$$C = (a' - a_\infty)^2 + a''^2$$

IV. RESULTS AND DISCUSSION

The values of dielectric constants,Higasi's parameters for different concentrations of 1-butanol and 1-propanol in

ISSN:0971-1260

Vol-22-Issue-10-November-2019

(Benzene+Ethylenediamine) at 303K,313K and 323K are reported in table 1 and table 2. Our results show that ε_{0m} value is higher than in pure liquids in benzene. This may be attributed due to the longer size of the molecules. Similar reports are given by Helambe et al.[9]. For both the systems the 'α' value is finite with for all concentrations and decrease with rise in temperatures. This implies that more than one relaxation processes exists. This may be due to the fact that at high temperature, molecular rotations of solute molecules become faster and uniform in the solution [10].A similar results was reported by Kalaivani et al. [11].From table 3, it

Table.1 Values of ε_m, ε_∞, ε', ε'', ρ and η at different temperatures.

ISSN:0971-1260

Vol-22-Issue-10-November-2019

Temp. (K)	Concentration of n-Propanol in (Benzene+ Ethylenediamine)	ε_m	ε_∞	ε'	ε''	ρ g/cc	$\eta x 10^{-2}$ Pa
303	0	2.8040	2.2061	2.5001	0.1910	0.8825	1.6370
	0.33	2.8850	2.2043	2.4586	0.1871	0.8814	1.6420
	0.50	2.9660	2.2014	2.4165	0.2081	0.8776	1.6390
	0.67	2.9120	2.1951	2.4441	0.2067	0.8740	1.6200
Temp. (K)							
303							
313							
323							
	1	2.7770	2.1624	2.4783	0.1854	0.8716	1.5850
313	0	2.7770	2.1969	2.5011	0.1886	0.8381	1.2940
	0.33	2.8580	2.1945	2.4599	0.1861	0.8355	1.2970
	0.50	2.9390	2.1889	2.4173	0.2056	0.8330	1.2940
	0.67	2.8850	2.1795	2.4455	0.1972	0.8306	1.2860
	1	2.7500	2.1474	2.4820	0.1845	0.8295	1.2520
323	0	2.7500	2.1889	2.5026	0.1845	0.8092	1.1010
	0.33	2.8310	2.1863	2.4610	0.1850	0.8078	1.1300
	0.50	2.9120	2.1830	2.4182	0.2043	0.8066	1.1290
	0.67	2.8580	2.1742	2.4464	0.1959	0.8062	1.1250
	1	2.7230	2.1383	2.4840	0.1830	0.8024	1.0660

ISSN:0971-1260

Vol-22-Issue-10-November-2019

System	Concen-tration	α			τ_0 (ps)			τ_1 (ps)			τ_2 (ps)		
		303 K	313 K	323 K	303 K	313 K	323 K	303 K	313 K	323 K	303 K	313 K	323 K
1-Butanol in (Benzene+ Ethylene diamine)	0	0.23	0.24	0.24	18.19	15.94	13.83	12.09	10.86	10.12	25.17	24.11	22.10
	0.33	0.28	0.27	0.26	23.01	19.92	17.31	12.34	11.51	10.91	30.87	28.59	26.18
	0.50	0.31	0.31	0.33	41.70	37.34	33.72	14.83	13.74	12.87	43.99	41.82	40.04
	0.67	0.31	0.31	0.31	27.52	24.30	21.53	12.22	11.68	11.15	35.62	33.35	31.28
	1	0.26	0.24	0.19	12.97	11.21	9.92	9.55	9.02	8.66	22.02	19.56	16.86
1-Propanol in (Benzene+ Ethylene diamine)	0	0.23	0.24	0.24	18.19	15.94	13.83	12.09	10.86	10.12	25.17	24.11	22.10
	0.33	0.30	0.31	0.31	31.33	27.40	23.92	13.31	12.39	11.67	37.57	35.26	32.97
	0.50	0.24	0.27	0.27	43.25	39.79	36.33	17.82	16.11	15.18	43.53	41.83	39.84
	0.67	0.26	0.30	0.30	33.41	30.08	26.85	15.05	13.11	12.47	37.31	36.74	34.63
	1	0.28	0.27	0.26	16.79	13.97	12.04	10.42	9.61	9.08	26.56	23.94	21.53

Table.2 Values of α,τ_0,τ_1, and τ_2 at different temperatures.

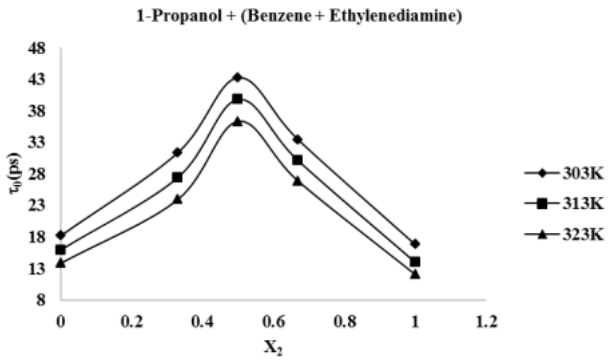


Fig.2 Variation of τ_0 with X_2

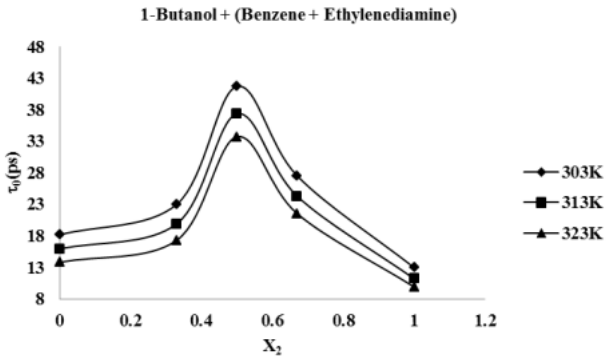


Fig.3. Variation of τ_0 with X_2

As concentration of alcohol increases, number of alcohol molecules also increases. This may be the reason for the enhancement of hetero association. τ_1 and τ_2 values for all the mixtures at all the studied temperatures have a non-linear variation with concentration of alcohol. This non-linear variation confirms the solute-solute interaction [12]. It was concluded that high viscosities provide larger can be seen that the most probable relaxation time (τ_0) value for the mixtures is greater than the corresponding value of the pure liquids. It indicates that the presence of strong hetero interaction between alcohol and amine. This trend exists in both the systems taken for investigation at all the studied temperatures as shown in figure 2&3.The relaxation time due to group rotation (τ_1) gives information in both the systems indicates

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Vol-22-Issue-10-November-2019

that the existence intramolecular interactions. Value of τ_1 decreases with rise of temperature. This may be due to the hindrance offered due to the thermal agitations. In the mixtures containing 1-propanol, τ_1 value is greater than in mixtures containing 1-butanol. Value of τ_2 reflects the overall size of the molecules. τ_2 value shows a non-linear variation with the concentration of alcohol. In all the mixtures the maximum value of τ_2 occurs at equimolar concentration of alcohol. This shows that at these concentrations, the aggregates have a large size droplet diameters and high penetration of the fuel. It leads hinders vaporization, favoring the formation of large diameter droplets and causing incomplete combustion due to the high penetration of the fuel, hindering cold starts and increasing the emission of unburned hydrocarbons (HCs) and particulate matter (PM). But at high temperature the size of the molecules reduced. It shows that shortened ignition delay and improved the combustion process [13, 14].

V.CONCLUSION

For three different temperatures, values of different dielectric parameters for the multifunctional fuel additives system 1-butanol and 1-propanol in (Benzene+Ethylenediamine) at various concentrations are reported.The nature of molecular association between the components is identified and results are interpreted. But at high temperature the size of the molecules reduced. It shows that shortened ignition delay and improved the combustion process when this added with diesel fuel. It can be concluded that the addition of oxygenates and corrosion inhibitor had reduced the exhaust emissions of engine.

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