FT-IR, molecular interactions and antibacterial studies of binary organic liquid mixtures of Geranyl acetate and Amyl alcohol at (303.15-318.15) K

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Abstract: Densities and ultrasonic speeds have been measured over the whole composition range for binary liquid mixtures of geranyl acetate with Amyl alcohol using a single crystal 2MHz ultrasonic interferometer at T = (288.15, 293.15, 298.15, 303.15, and 308.15) K and atmospheric pressure to evaluate these binaries' behaviour. These data have calculated excess molar volume, deviation in adiabatic compressibility, excess free volume, excess intermolecular free length, excess gibs energy and excess enthalpy. These excess properties have been fitted with the Redlich– Kister type polynomial equation to get their coefficients and standard deviations, which provide a base for discussing the forces operating in solutions, FT-IR and the antibacterial activity of liquid combinations and individual chemicals were studied.

Keywords: Geranyl acetate; molecular interactions; Amyl alcohol; viscosity ; density ; FTIR;Antibacterial activity.

1. Introduction

Understanding the thermodynamic characteristics of binary liquid mixtures has effectively explained the structural interactions of constituents [1-9]. Many researchers have shown the fundamental role of the molecular details of the solvent species to determine the specific interactions responsible for macroscopic, thermodynamic, and other related properties in non-electrolyte solutions. Knowledge about the density and viscosity of binary liquid mixtures is essential for understanding the behaviour of liquids. Volumetric properties of liquids are a powerful tool in understanding molecular systems' nature and physicochemical behaviour. Esters play a vital role in medicinal, industrial, chemical and biological areas. Due to their

biodegradability, they are an essential constituent of marine engine oils, drugs, inks, cosmetics, hydraulic fluids etc.

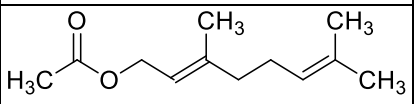
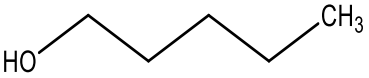
Moreover, esters are widely helpful in the food industry for their aroma and flavours. They also impart desired thermos plasticity to polymers. Many researchers have described the role of thermo dynamic excess properties with the pattern of molecular interaction between molecules of esters with alkanols [10-18]. When binary or more complex mixtures are used as solvent media, specific solvent-to-solvent interactions can modify the pure liquids' structural properties and molecular arrangement. Thus, the knowledge of the structure of mixed solvent systems becomes an essential prerequisite to interpreting and understanding the interaction patterns between ions, ion pairs and ionic aggregates, and bulk solvent molecules. In principle, the interaction between the molecules can be established by studying the characteristics of abrupt departure from the ideal behaviour of some physical properties, like volume, compressibility, viscosity, etc. The ultrasonic technique has been adequately employed to investigate the properties of many substances to understand the nature of molecular interactions in pure liquid mixtures and ionic interactions in electrolytic solutions. Though molecular interaction studies can be best carried out through spectroscopic methods, other no-spectroscopic techniques such as dielectric, ultrasonic velocity, and viscosity measurements have been widely used in interactions and structural aspect evaluation studies. Many workers have extensively studied complex formation in liquid mixtures using optical and ultrasonic techniques [19–21]. The formation of hydrogen bonds in solutions and its effect on the physical properties of the mixtures have received much attention. Hydrogen bonding plays a vital role in fundamental sciences and industrial applications. Although many experimental and theoretical studies have been directed towards understanding hydrogen bonding, it remains an active research area. Knowledge of the physicochemical properties of liquid mixtures formed by two or more components associated with hydrogen bonds is vital from theoretical and process design aspects. Acyclic monoterpene alcohol, geraniol (trans-3,7-dimethyl-2,6-octadien-1-ol) occurs in essential oils of plants like lemongrass, rose, and geranium. Geranyl acetate is a natural organic compound. It's a taintless liquid with a pleasant flowery or gooey rose aroma. Geranyl acetate exists naturally in more than 80 essential oils, including Ceylon citronella, palmarosa, lemon grass, geranium, coriander, sassafras, etc. Geranyl acetate is prepared by esterification of acetic acid and geraniol in large-scale industries. It is used as scents for detergents and creams and as a seasoning component. More recent, more marketable uses for geraniol have been suggested,

including use as an excellent replacement for gasoline and as a medicinal agent for treating cancer, inflammation, and pain.

2. Materials and Experiments

Sigma Aldrich Pvt.Ltd., India, offers geranyl acetate, while Otto Chemie Pvt.Ltd., India, supplies Amyl alcohol. These chemicals were not subjected to any purification method before the experiment. Table 1 lists the liquids sources, purity, and chemical composition. The liquids were distilled before use and combined in exact proportions using a burette. They kept a side to stand still for five or six hours until thermal equilibrium was attained, then later measured. The formation of bubbles inorganic liquids, which distort the density measurement, is usually caused by dissolved gases. All liquids were degassed prior to reading to avoid difficulties. In this study, all materials purchased were Sigma-Aldrich AR grade and borosilicate glassware. The specific gravity bottle and Ostwald viscometer were used to determine the Density and Viscosity of liquid compounds to calibrate the viscometer in milligrams/ml with 3D Millipore water [22]. In the Ostwald viscometer, the flow time of viscous liquids is measured to the nearest 0.01second. Tests were performed using a Japan-made Shimadzuel electronic balance, a borosilicate glass instrument with a sensitivity of +0.001g. Mittal Enterprises, New Delhi, offers single crystal variable path fixed frequency interferometers for measuring the ultrasonic velocities of pure components and their mixtures. (Form- F05). The ultrasonic velocity measurements were performed at a fixed frequency of 2MHz [23- 24]. Less than 0.1% is assumed to be the average deviation in the recorded sound velocity. Proportional temperature controllers and microprocessor-assisted circulating water baths(supplied by Mac, NewDelhi) are used to manage temperatures within +0.01K so that density can be measured. Degree, viscosity and ultrasonic speed. Bruker FT-IR spectrometer(Germany), alpha-T with multimeter module, is used to study FT-IR spectra of the pure liquid mixture and binary liquid mixture. Chemical Samples were prepared by combining Amylalcohol and geranyl acetate in a 1:1 ratio. Spectra in the range 4000-400 cm^{-1} at 303.15K were recorded using a droplet of homogeneous liquid mixture. To conduct further experiments, 30ml of a binary mixture containing geranyl acetate and Amyl alcohol was prepared, with different volumes of 5ml each [25].

Table 1. Details about the samples

Name of the chemical	**Source of the chemical**	**Mass fraction purity**	**CAS Number**	**Molar Mass**	**Structure**
Geranyl acetate	Sigma-Aldrich Pvt. Ltd. India.	≥0.98	105-87-3	196.29	
Amyl alcohol	Otto chemie Pvt. Ltd. India	≥0.99	71-41-0	88.15	

3. Results and discussion

The current study describes new experimental findings on density and sound speed for binary geranyl acetate mixtures. Additionally, different thermodynamic properties include excess velocity, excess adiabatic compressibility, excess molar volume, excess internal pressure, excess intermolecular free length, excess Viscosity, excess impedance, excess free volume, excess free volume, excess Gibb's free energy, and excess enthalpy have been computed from the measured data. The derived excess parameters were fitted to the Redlich- Kister polynomial equation in order to calculate the standard deviation between the experimental and calculated values for binary mixtures geranyl acetate (1) and Amyl alcohol (2) for T = (303.15 -318.15) K. The results regarding the existing interactions between the mixtures under investigation have been interpreted.

The excess molar volumes (V^E) have been evaluated from density using

$$V^E = (x_1M_1 + x_2M_2)/\rho_m - (x_1M_1/\rho_1 + x2M2/\rho_2)$$

where ρ_m is the density of the mixture; x1, M1, and ρ_1 and x2, M2, and ρ_2 are the mole fraction, molar mass, and density of pure components, respectively.

The excess or deviation properties ΔY are fitted by the method of nonlinear least-squares to the fourth-order Redlich-Kister type polynomial.

$$\Delta Y = x_1x_2\sum A_i (x_1 - x_2)^i$$

Table2: Density (ρ), viscosity (η) and Velocity (U) of the pure geranyl acetate studied in this work at (303.15-318.15) K and 0.1 MPa using a single crystal 2MHz ultrasonic interferometer

Parameter	**303.15K**		**308.15K**		**313.15K**		**318.15K**	
	Expt.	Lite.	Expt.	Lite.	Expt.	Lite.	Expt.	Lite.
Density(ρ) kg m^{-3}	1672.49	-	1667.27	-	1661.83	-	1656.23	-
Viscosity (η) N s m^{-2}	5.6067	-	4.8082	-	4.1885	-	3.6780	-
Velocity(U) m s^{-1}	1386.04	-	1368.66	-	1351.32	-	1334.12	-

The degree uncertaintiesabove calculated parameters are**(ρ)** ±0.1 kgm^{-3}, **(η)**±2·10^{-6} Nsm^{-2} and **(U)** ±0. 3ms^{-1}respectively.

Table.3. Using a single crystal 2MHz ultrasonic interferometer, the density (ρ), viscosity (η), and velocity (U) of pure Amyl alcohol were measured in this study at (303.15-318.15) K and 0.1 MPa.

Parameter	**303.15K**		**308.15K**		**313.15K**		**318.15K**	
	Expt.	**Lite.**	**Expt.**	**Lite.**	**Expt.**	**Lite.**	**Expt.**	**Lite.**
Density (ρ) kg/m^3	807.06	806.7[27]	803.33	805.2[26] 784.6[28]	801.56	802.6[26]	797.75	-
Viscosity (η) Ns/m^2	3.107	2.9580[26]	2.7342	2.9016[26]	2.3240	2.3923[26]	2.0027	-
Velocity (U) m/s	1265.6	1268.0[26]	1234.9	1225.1[26]	1220.1	1218.4[26]	1210.4	-

The degree uncertaintiesabove calculated parameters are**(ρ)** ±0.1 kgm^{-3}, **(η)**±2·10^{-6} Nsm^{-2} and **(U)** ±. 3ms^{-1}respectively.

Table 4: Ultrasonic Velocity (U), density (ρ), viscosity (η), Adiabatic compressibility (βad), Inter Molecular Free Length (L_f), Molar Volume (V_m), Rao's Constant (R) and Wada's Constant (W) for binary mixtures geranyl acetate (1) and Amy alcohol (2) for T = (303.15 - 318.15) K

Mole fraction (X_1)	**Mole fraction (X_2)**	**Velocity m/sec**	**Density Kg/m^3 (ρ)**	**Viscosity Nsm^{-2} (η)**	**Ad. Comp. 10^{-10}**	**Int. Mol. Free length**	**Mol. Vol. (V_m)**	**Rao'sConstnt (R)**	**Wada's Constant (W)**

		(U)			$N^{-1}.m^2$ (β_{ad})	10^{-10} m (L_f)			
T= 303.15 K									
0.0000	1.0000	1265.6	807.06	3.107	7.7357	5.7712	109.22	5.4838	8.1543
0.1569	0.8430	1285.7	951.29	3.5236	6.3595	5.2327	110.5	5.5771	8.4839
0.3175	0.6824	1305.7	1095.5	3.9402	5.3538	4.8011	111.81	5.6723	8.7980
0.482	0.5179	1325.8	1239.7	4.3568	4.5888	4.4449	113.15	5.7696	9.1017
0.6505	0.3495	1345.9	1383.9	4.7734	3.9888	4.1442	114.52	5.8688	9.3983
0.8231	0.1769	1366.0	1528.2	5.1900	3.5070	3.8858	115.93	5.9703	9.6903
1.0000	0.0000	1386.04	1672.4	5.6066	3.1124	3.6607	117.37	6.0739	9.9794
T=308.15 K									
0.0000	1.0000	1234.9	803.33	2.7342	8.1629	5.9856	109.73	5.4644	8.1295
0.1569	0.8430	1257.2	947.32	3.0798	6.6788	5.4142	110.99	5.5600	8.4618
0.3175	0.6824	1279.5	1091.3	3.4254	5.5973	4.9565	112.27	5.6575	8.7786
0.482	0.5179	1301.8	1235.3	3.7710	4.7770	4.5789	113.59	5.7569	9.0849
0.6505	0.3495	1324.1	1379.3	4.1166	4.1354	4.2603	114.94	5.8582	9.3840
0.8231	0.1769	1346.4	1523.3	4.4622	3.6215	3.9868	116.32	5.9617	9.6784
1.0000	0.0000	1368.7	1667.3	4.8078	3.2018	3.7487	117.73	6.0672	9.9699
T=313.15 K									
0.0000	1.0000	1234.9	801.56	2.324	8.1809	6.0493	109.97	5.4764	8.1449
0.1569	0.8430	1254.3	944.94	2.6348	6.7265	5.4853	111.25	5.5689	8.4732
0.3175	0.6824	1273.7	1088.3	2.9455	5.6638	5.0334	112.56	5.6633	8.7861
0.482	0.5179	1293.1	1231.7	3.2563	4.8554	4.6604	113.9	5.7597	9.0884
0.6505	0.3495	1312.5	1375.1	3.567	4.2215	4.3455	115.27	5.8580	9.3836
0.8231	0.1769	1331.9	1518.5	3.8778	3.7123	4.0750	116.68	5.9585	9.6740
1.0000	0.0000	1351.3	1661.8	4.1885	3.2953	3.8393	118.12	6.0612	9.9615
T=318.15 K									
0.0000	1.0000	1210.4	797.75	2.0027	8.5561	6.2450	110.5	5.4659	8.1315
0.1569	0.8430	1231	940.83	2.2819	7.0139	5.6543	111.76	5.5595	8.4611
0.3175	0.6824	1251.6	1083.9	2.5611	5.8891	5.1811	113.05	5.6548	8.7751
0.482	0.5179	1272.3	1227.0	2.8403	5.0351	4.7907	114.37	5.7521	9.0785
0.6505	0.3495	1292.9	1370.1	3.1195	4.3666	4.4614	115.72	5.8513	9.3745
0.8231	0.1769	1313.5	1513.2	3.3987	3.8305	4.1786	117.1	5.9525	9.6657
1.0000	0.0000	1334.1	1656.2	3.6779	3.3923	3.9323	118.52	6.0559	9.9539

Table 5. Free Volume (V_f), Acoustic Impedance (Z), Internal Pressure (Π), Gibb's Energy (G^E), Enthalpy (H) and Relaxation Time (T)for binary mixtures geranyl acetate (1) andAmyl alcohol(2) for T = (303.15 -318.15) K

Mole fraction (X1)	Mole fraction (X2)	Free Volume (Vf)	Acoustic Impedance (Z)	Internal pressure (π)	Gibb's Energy (G^E)	Enthalpy (H)	Relaxation time (τ)
T= 303.15 K							
0.0000	1.0000	0.2429	1.0214	761.76	0.1138	83.203	3.2047
0.1569	0.8430	0.2682	1.2230	731.36	0.1136	80.816	2.9878
0.3175	0.6824	0.2920	1.4305	705.36	0.1133	78.867	2.8127
0.4820	0.5179	0.3149	1.6437	682.39	0.1131	77.212	2.6656
0.6505	0.3495	0.3373	1.8627	661.6	0.1129	75.767	2.5387
0.8231	0.1769	0.3595	2.0875	642.46	0.1128	74.478	2.4268

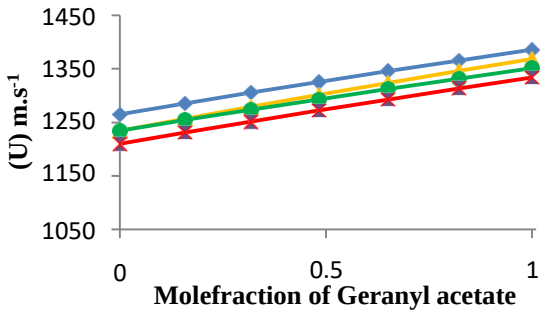
1.0000	0.0000	0.3816	2.3181	624.6	0.1126	73.307	2.3267
T=308.15 K							
0.0000	1.0000	0.2836	0.9920	733.09	0.1155	80.443	2.9759
0.1569	0.8430	0.3174	1.1910	700.72	0.1152	77.772	2.7426
0.3175	0.6824	0.3496	1.3963	673.38	0.1149	75.603	2.5564
0.482	0.5179	0.3806	1.6081	649.48	0.1147	73.775	2.4019
0.6505	0.3495	0.4111	1.8263	628.06	0.1144	72.188	2.2698
0.8231	0.1769	0.4413	2.0509	608.51	0.1142	70.781	2.1547
1.0000	0.0000	0.4716	2.2819	590.43	0.1141	69.513	2.0525
T=313.15 K							
0.0000	1.0000	0.3619	0.9898	685.83	0.1167	75.423	2.5349
0.1569	0.8430	0.3997	1.1852	658.4	0.1165	73.248	2.3630
0.3175	0.6824	0.4353	1.3862	634.99	0.1162	71.475	2.2243
0.4820	0.5179	0.4695	1.5927	614.32	0.1160	69.971	2.1080
0.6505	0.3495	0.5029	1.8048	595.63	0.1158	68.659	2.0077
0.8231	0.1769	0.5359	2.0224	578.43	0.1157	67.489	1.9194
1.0000	0.0000	0.569	2.2456	562.4	0.1155	66.428	1.8403
T=318.15 K							
0.0000	1.0000	0.4390	0.9656	651.26	0.1183	71.963	2.2847
0.1569	0.8430	0.4823	1.1582	626.41	0.1180	70.007	2.1340
0.3175	0.6824	0.5232	1.3567	605.02	0.1178	68.396	2.0110
0.4820	0.5179	0.5626	1.5611	585.98	0.1176	67.017	1.9068
0.6505	0.3495	0.6013	1.7713	568.66	0.1174	65.804	1.8162
0.8231	0.1769	0.6398	1.9875	552.64	0.1172	64.715	1.7358
1.0000	0.0000	0.6783	2.2096	537.65	0.1171	63.720	1.6635

Table 6. Excess Velocity (U^E), Excess Adiabatic compressibility ($\Delta\beta_{ad}$), Excess Intermolecularfree length (L_f^E), Excess Impedance (Z^E), Excess Molar volume (V_m^E), Excess Free volume (V_f^E), Excess Viscosity ($\Delta\eta$), Excess Internal pressure (Π^E), Excess Gibb's free energy (ΔG^E) and Excess Enthalpy (H^E).for binary mixtures geranyl acetate (1) andAmyl alcohol(2) for T = (303.15 -318.15) K

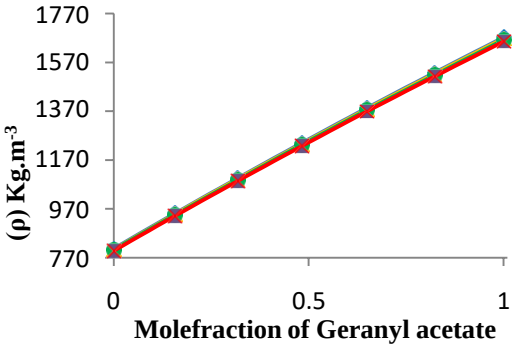
Mole fraction (X1)	U^E	$\Delta\beta_{ad}$	L_f^E	Z^E	V_m^E	V_f^E	$\Delta\eta$	Π^E	ΔG^E	H^E
T=303.15 K										
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1569	1.1743	-0.6507	-0.2072	-0.0018	-0.0441	0.0035	0.0244	-8.8846	0.0008	-0.834
0.3175	1.9012	-0.9138	-0.2999	-0.0027	-0.0728	0.0050	0.0395	-12.843	0.0013	-1.1939
0.4820	2.1644	-0.9184	-0.3090	-0.0028	-0.0910	0.0051	0.0449	-13.253	0.0014	-1.2207
0.6505	1.9473	-0.7394	-0.2541	-0.0022	-0.0984	0.0041	0.0404	-10.936	0.0012	-0.9984
0.8231	1.232	-0.4233	-0.1482	-0.0012	-0.0843	0.0024	0.0256	-6.4054	0.0007	-0.5799
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
T=308.15 K										
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1569	1.277	-0.7046	-0.2199	-0.0037	-0.0531	0.0043	0.0053	-9.9541	0.0007	-0.9536
0.3175	2.0669	-0.9885	-0.3180	-0.0058	-0.0871	0.0062	0.0076	-14.363	0.0011	-1.3651
0.4820	2.3525	-0.9926	-0.3276	-0.0062	-0.1085	0.0063	0.0077	-14.794	0.0012	-1.3955
0.6505	2.1159	-0.7986	-0.2694	-0.0053	-0.1167	0.0051	0.0063	-12.183	0.0010	-1.1410
0.8231	1.3383	-0.4568	-0.1571	-0.0031	-0.0995	0.0029	0.0036	-7.1221	0.0006	-0.6624
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
T=313.15 K										
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

0.1569	1.1278	-0.6874	-0.2171	-0.0017	-0.0695	0.0053	0.0181	-8.0486	0.0008	-0.7621
0.3175	1.8256	-0.9652	-0.3139	-0.0026	-0.1122	0.0076	0.0292	-11.628	0.0013	-1.0912
0.4820	2.0783	-0.9699	-0.3234	-0.0026	-0.1378	0.0077	0.0333	-11.994	0.0014	-1.1153
0.6505	1.8696	-0.7808	-0.2660	-0.0021	-0.1462	0.0063	0.0299	-9.8918	0.0011	-0.9120
0.8231	1.1828	-0.4469	-0.1551	-0.0012	-0.1230	0.0036	0.0189	-5.7914	0.0007	-0.5295
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
T=318.15 K										
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1569	1.1757	-0.7306	-0.2273	-0.0029	-0.0843	0.0057	0.0159	-6.9931	0.0009	-0.6610
0.3175	1.9028	-1.0252	-0.3286	-0.0045	-0.1351	0.0081	0.0257	-10.123	0.0014	-0.9473
0.4820	2.1657	-1.0295	-0.3384	-0.0048	-0.1650	0.0081	0.0293	-10.461	0.0015	-0.9695
0.6505	1.9478	-0.8283	-0.2782	-0.0040	-0.1740	0.0065	0.0263	-8.6437	0.0013	-0.7936
0.8231	1.2319	-0.4738	-0.1622	-0.0024	-0.1454	0.0037	0.0166	-5.0697	0.0008	-0.4611
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

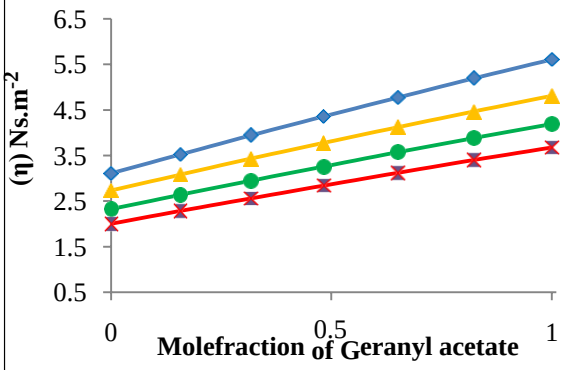
Graphs



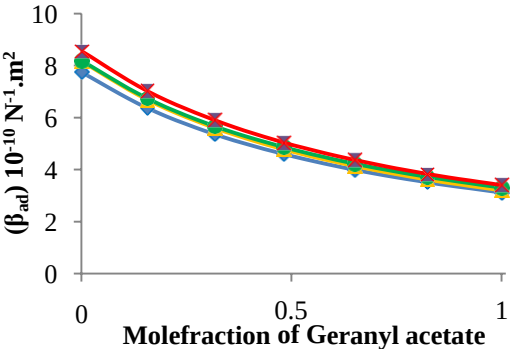
Graph-1: Ultrasonic velocity Vs Mole fraction of Geranyl acetate (X_1)



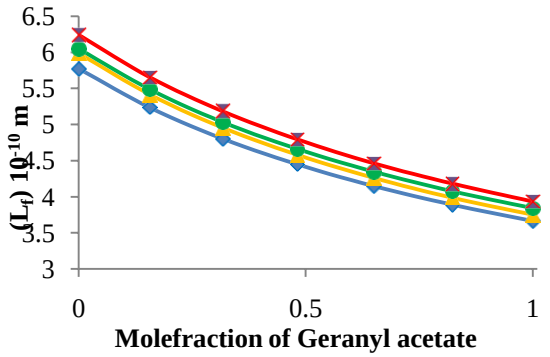
Graph-2: Density Vs Mole fraction of Geranyl acetate (X_1)



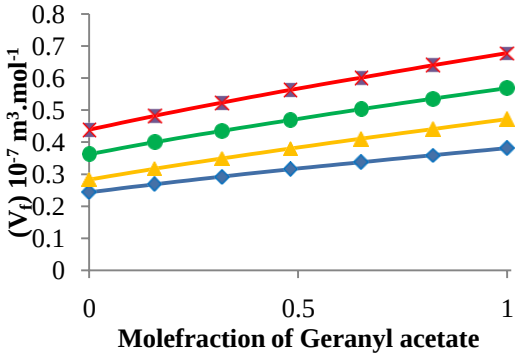
Graph-3: Viscosity Vs Mole fraction of Geranyl acetate (X_1)



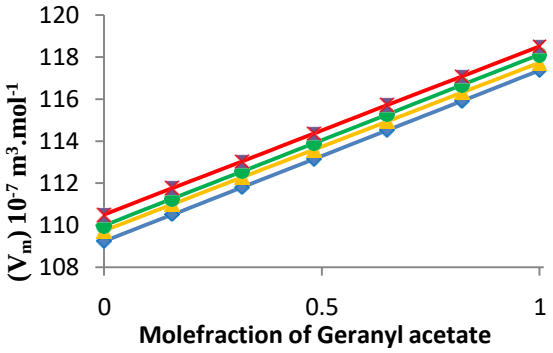
Graph-4: Adiabatic Compressibility Vs Mole fraction of Geranyl acetate (X_1)



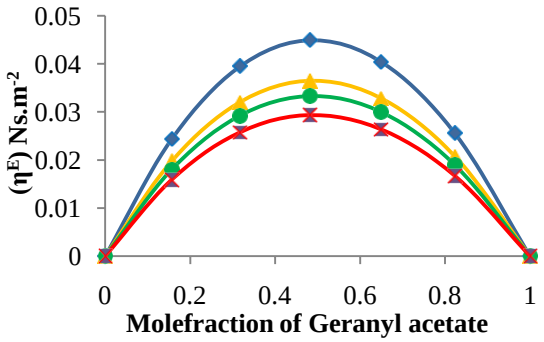
Graph -5: Intermolecular Free Length Vs Mole fraction of Geranyl acetate(X_1)



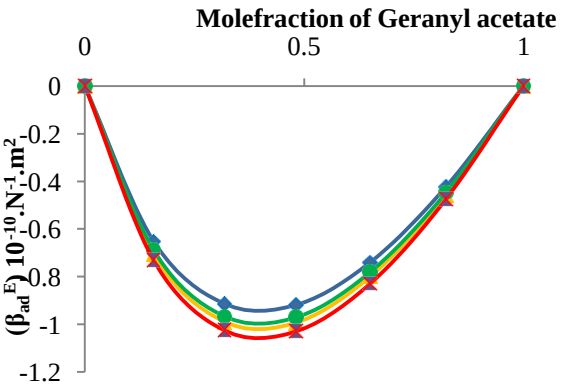
Graph -6: Free volume Vs Mole fraction of Geranyl acetate (X_1)



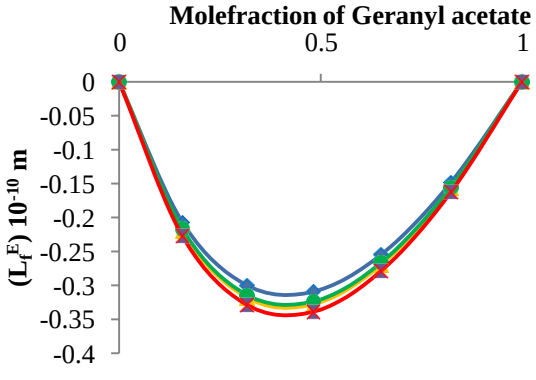
Graph -7: Molar Volume Vs Mole fraction of Geranyl acetate
(X_1)



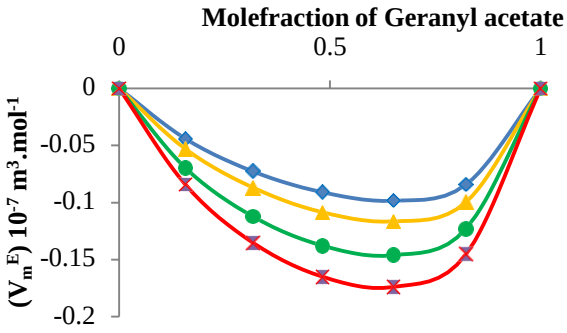
Graph -8: Deviation in Viscosity Vs Mole fraction of Geranyl acetate (X_1)



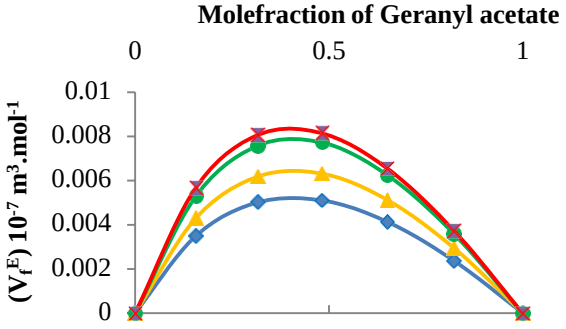
Graph -9: Excess adia. Compressibility Vs Mole fraction of Geranyl acetate(X_1)



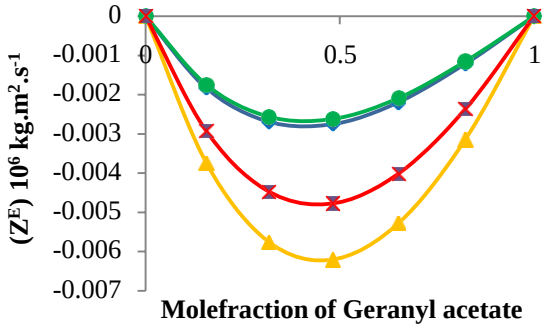
Graph -10: Excess Intermolecular Free Length Vs Mole fraction of Geranyl acetate (X_1)



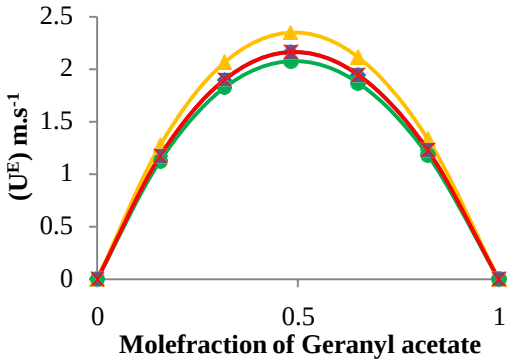
Graph -11: Excess Molar Volume Vs Mole fraction of Geranyl acetate (X_1)



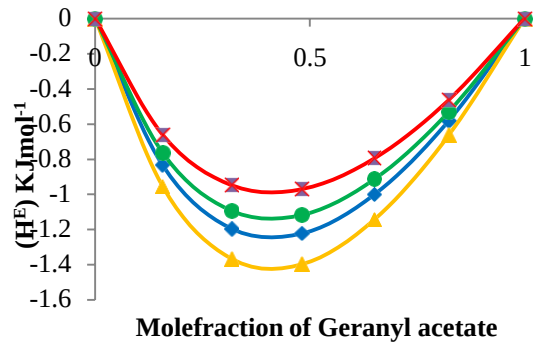
Graph -12: Excess free volume Vs Mole fraction of Geranyl acetate(X_1)



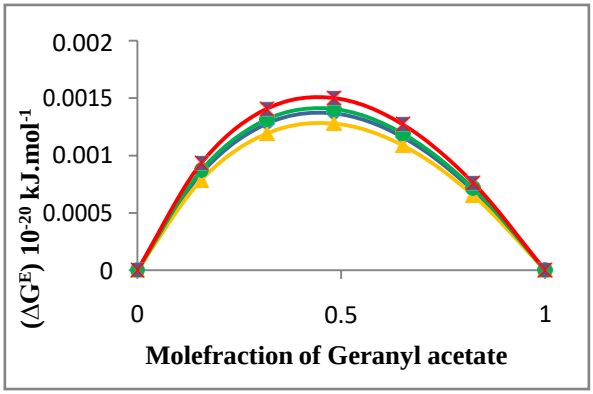
Graph -13. Excess acoustic impedance Vs Mole fraction of Geranyl acetate(X_1)



Graph -14. Excess velocity Vs Mole fraction of Geranyl acetate (X_1)



Graph -15. Excess Enthalpy Vs Mole fraction of Geranyl acetate(X_1)



Graph -16. Excess Gibbs energy Vs Mole fraction of Geranyl acetate(X_1)

The experimentally measured values of density (ρ), viscosity (η), ultrasonic velocity (U), and computed values of adiabatic compressibility (β), acoustic impedance (Z), free length (Lf), free volume (Vf), internal pressure (π), relaxation time (τ), Gibbs free energy (ΔG) for a binary mixture of Geranyl acetate and Amyl alcohol at 303.15, 308.15,313.15 and 318.15 K are listed in Table 3 and 4. From Table 3, it can be seen that the density of the binary mixtures increases as the Geranyl acetate fraction increases. Geranyl acetate's viscosity increases with increasing mole fraction by strengthening intermolecular interactions between the components. Across all compositions of liquid mixtures, Density and Viscosity decreased as temperature increased. Thermally agitating molecules loosen the intermolecular forces in an aqueous system [29]. The ultrasonic velocity increases with the concentration of Geranyl acetate (graph.1). It reveals the structural changes occurring in the mixtures resulting in the strengthening of intermolecular forces. A least squares method was used to determine ultrasonic velocity standard deviations, which are shown in Table 6. It can be deduced from the decreasing adiabatic Compressibility of Geranyl acetate with increasing concentration that strong interactions between molecules result in less compressibility [30]. Layer by layer in a liquid system, the pressure changes when an ultrasonic wave travels. Consequently, ultrasonic velocity and density vary with liquid mixture concentration. The product of the density and ultrasonic velocity is called acoustic impedance (Z). This study found that acoustic impedance increased as Geranyl acetate concentration increased. According to this observation, molecular interactions exist between liquids [31]. The intermolecular free length (L_f) is an important determinant of molecular interaction. It depends upon the adiabatic compressibility. There is a possibility ofdipole–dipole interaction between the amyl alcohol molecules and hydrogen bonds with the Geranyl acetate molecules in the mixture. The increase in temperature however makes the free length to increase as expected due to the thermal expansion of the liquids.In this study, free length reflects the trend of adiabatic compressibility as listed in Tables 3 and 4.The upward trend in free volume suggests that the hydroxyl and carbonyl groups in Amyl alcohol and geranyl acetate can generate dipoles together, supporting the need for more space between the components. As shown in Table 4, the internal pressure shows a reversal trend. As shown in Table 4, the internal pressure shows a reversal trend. The relaxation period, influenced by temperature and contaminants, is the period for the excitation energy to emerge as translational energy. The characteristic time of the relaxation process that creates dispersion should be disclosed in the system's dispersion of the speed of sound. The structural relaxation process is responsible for the relaxation

period, which is in the range of 10^{-12} seconds[32] And such a case,it is proposed that the cooperative process causes the molecules to reorganize themselves [33-36]. The reduction of Gibbs free energy (ΔG) with the Geranyl acetate concentrations in all the temperatures signifies the weak hydrogen bonding formed with Amyl alcohol at the higher concentration of Geranyl acetate. Examining the excess parameters rather than the actual values is crucial to clarify the nature of molecular interactions between the constituents of the liquid mixes. When temperature and concentration are combined with strong or weak interactions, non-ideal liquid mixtures behave significantly differently from linearly. The excess values of β_{ad}^{E}, τ^{E}, and ΔG^{E} are listed in Table 6. From the experimental excess parameters, the negative trend observed in β_{ad}^{E}, L_f^{E} and V_m^{E} shows the strong molecular interactions between geranyl acetate and Amyl alcohol. The broad peak in FT-IR confirmed the strong hydrogen bonding between geranyl acetate and Amyl alcohol.

Chart 1(a) shows a characteristic absorption at 1720 cm^{-1}, which is attributed to the stretching frequency of the C=O bond of the Geranyl acetate. The absorption band at 3333 cm^{-1}which is attributed to the stretching frequency of the free O-H bond in alcohol. The band at 2983 cm-1 and 2929 cm^{-1} stated the stretching frequency of the C-H bond in Geranyl acetate and Amyl alcohol. The frequency range at 1070 and 1050cm^{-1} belongs to the C-O stretching of pure Geranyl acetate and Amyl alcohol, respectively.

Chart 1(b) shows that the absorption bands at 1721 cm^{-1} are associated with the stretching frequency of C=O in the combination of Geranyl acetate and Amyl alcohol. The C=O stretching frequency increased from 1720cm^{-1} to 1721cm^{-1}. From the above, we conclude that molecular interactions are observed due to the slight variation obtained in C=O stretching frequency, which supports the intermolecular hydrogen bonding observed in a binary organic liquid mixture of Geranyl acetate and Amyl alcohol. As a result of the shifting of OH stretching vibration frequencies from lower to higher frequencies, FT-IR analysis can conclude that the hydrogen bonds present in mixtures are weak [46-51].

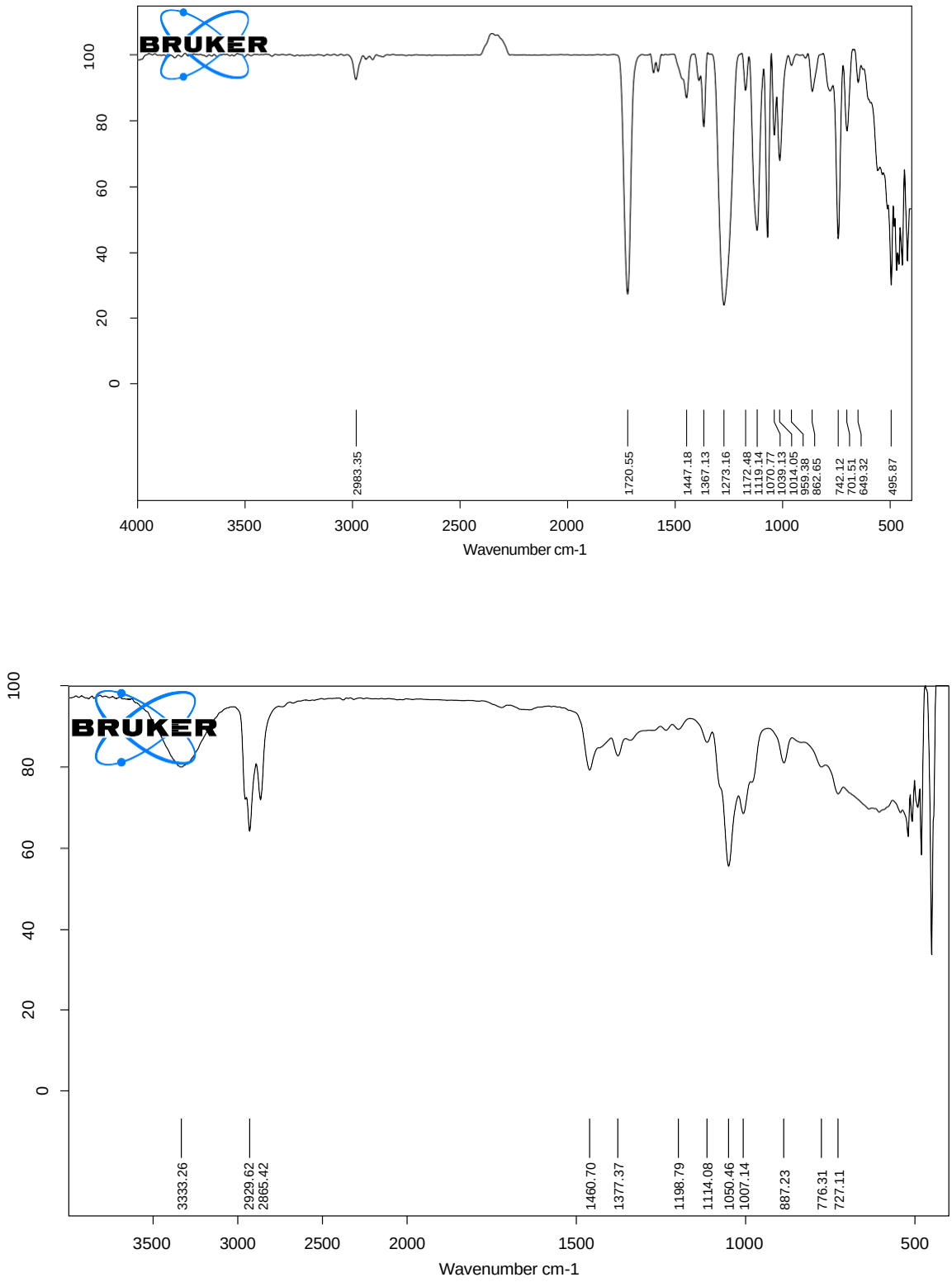


Chart1(a). FTIR spectrum of pure Geranyl acetate and pure Amyl alcohol.

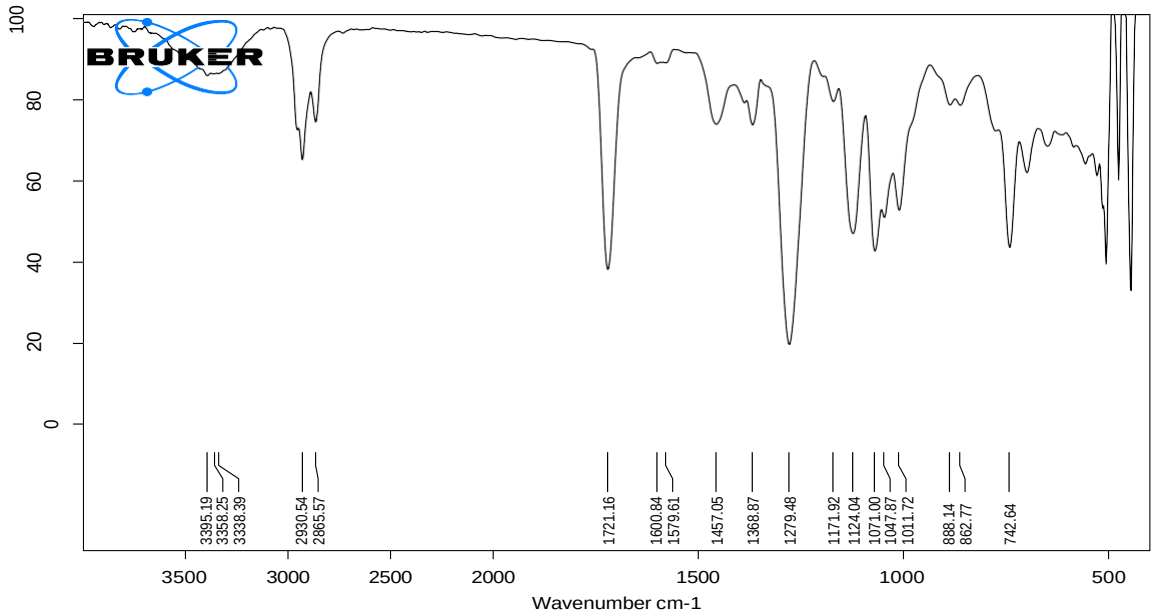
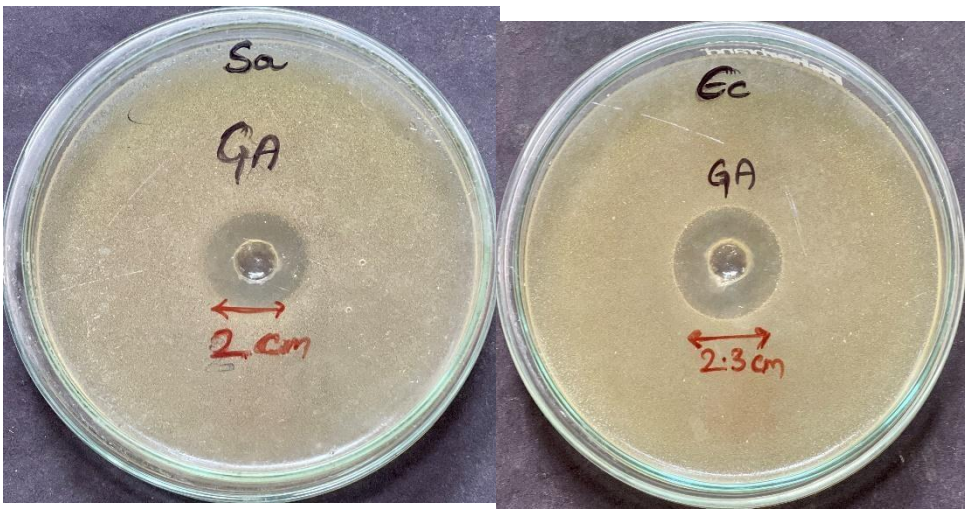
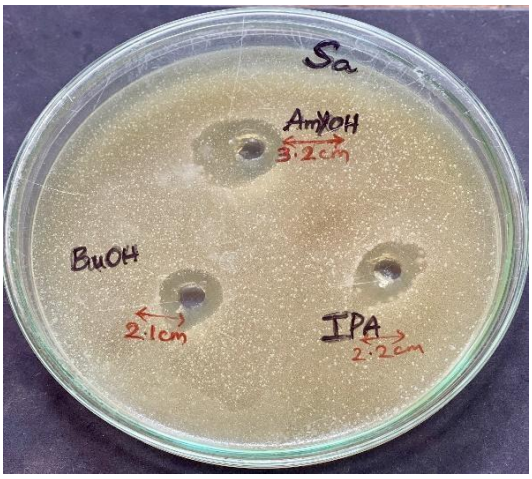


Chart 1(b). FTIR spectrum of Geranyl acetate + Amyl alcohol

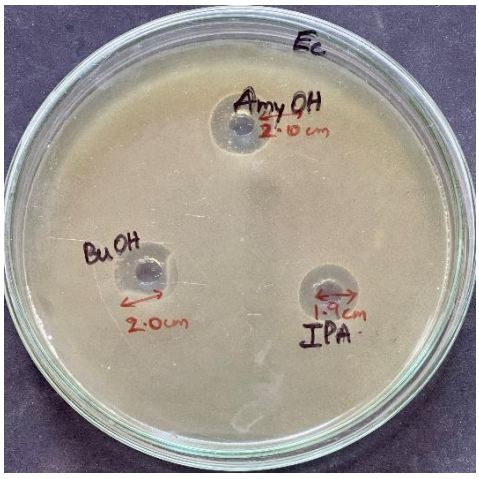
Fig 1: Antibacterial activity of Esters and binary mixtures (a,b) Geranyl acetate pure, (c,d) Amyl alcohol Pure (e) Geranyl acetate+ Amyl alcohol, (f) Geranyl acetate+ amyl alcohol. Geranyl acetate and Amyl alcohol mixture have been screened for antibacterial activity against certain bacteria. Staphylococcus aureus (gram +ve), and Escherichia coli (gram -ve) are used. Antibacterial screening is done by the well diffusion method.



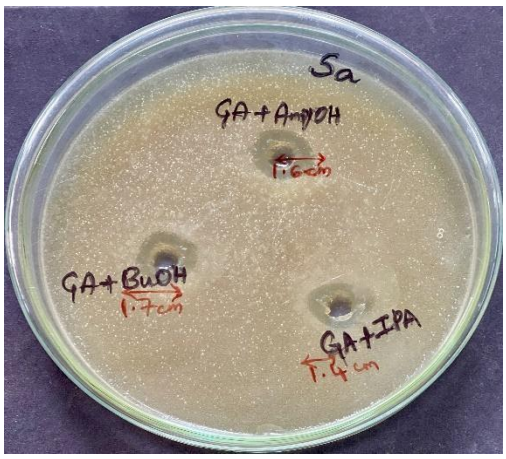
(a) Staphylococcus aureus **b) *Escherichia coli***



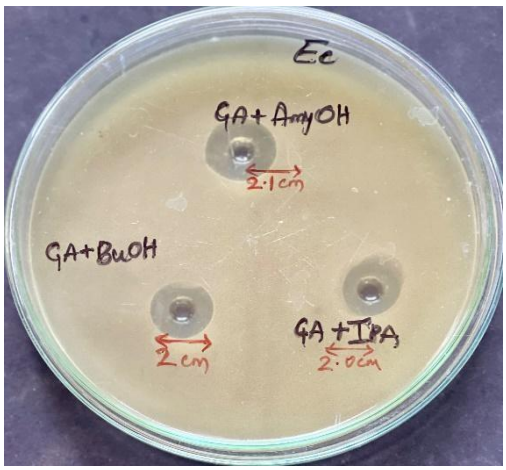
(c) *Staphylococcus aureus*



(d) *Escherichia coli*



(e) *Staphylococcus aureus*



(f) *Escherichia coli*

Fig 1: Antibacterial activity of binary mixtures (a,b) Geranyl acetate pure, (c,d) Amyl alcohol Pure (e) Geranyl acetate+ Amyl alcohol, (f) Geranyl acetate+ Amyl alcohol

Table 7. Antibacterial activities of Geranyl acetate, Amyl alcohol and binary mixture

Name of the sample	**Antibacterial activities (in cm) Zone of inhibition**	
	*S.aureus*zone (cm)	*E. coli* zone (cm)
Geranyl acetate	2.0	2.3
Amyl alcohol	3.2	2.0
Geranyl acetate + Amyl alcohol	1.6	2.1

The experimental data of pure and mixtures are presented in Table 7. The pure Geranyl acetate showed a zone of inhibition of 2.0cm and 2.3cm against both organisms, respectively. Amyl alcohol showed a zone of inhibition of 3.2cm against *Staphylococcus aureus and* 2.0cm against *E. coli*. The zone of inhibition distance of the mixture of Geranyl acetate and Amyl alcohol is 1.6 cm by E. *coli* and 2.1cm by S.*aures*. Compared to the antibacterial bioactivity of the mixtures, the individual components in a binary mixture were found to be decreased. The anti-microbial activity on coordination can be described by Overtone`s concept and chelation theory [40].

4. Conclusions

The experimental measurements determined the physical and acoustical parameters for the binary mixture of Geranyl acetate and Amyl alcohol at 303.15, 308.15, 313.15and 318.15 K. The calculated excess values and their sign show the specific hydrogen bonding interaction between the carbonyl group of Geranyl acetate and the hydroxyl group of Amyl alcohol. Moreover, sound velocity is 303.15 K > 308.15 K >313.15> 318.15 K. The FT-IR spectra confirm the formation of hydrogen bonding in the equimolar binary mixture systems. The bioactivity decreased from the individual compounds to the binary mixture.

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References

1. 1.Goralski P, Wasiak M, Bald A. J Chem. Eng.Data. 2002; 47(1):83-86.
2. Litovitz TA, Davis CM. Academic Press, New York.1965;282.
3. Moha-Ouchane M, Boned C, Xans P. Physica B. 1999;265(1-4):287-290.
4. Palaniappan Lakshmanan. Physica B. 2008;403(21-22):3887-3891.
5. Gokhan S, Ertunc A. Indian Academy of Sciences. 2006;66(2):435-446.
6. Bhawana S, Tripathi, Anjali A, Aashees A. Canadian J. Physics. 2010;88(4):283-292.

7. Kammerer K, Oswald G, Rezanova E, Silkenbaumer D, LichtenthalerRN. FluidPhase Equilib. 2000;167(2):223-241.
8. Nayakulu SVR, Venkateswar S, Reddy CS, Reddy DL. Phys.Chem. Liquids 2006;44(3):269-273.
9. Thirumaran S, Deepesh George. ARPN J. Eng. App.Sci.2009;4(4):1-11.
10. Anjali Awasthi, Aashees Awasthi. Thermochimica Acta. 2012; 537:57.
11. Amalendu Pal, Harsh Kumar, Ritu Maan, Harish Kumar Sharma. J Solution Chem. 2013; 42:1988.
12. Ortega J, Pena JA, Paz Andrade MI. J Chem. Eng Data. 1986; 39:1685.
13. Qin AJ, Hoffmann DE, Munk P. Czech. Chem. Commun. 1993; 58:2625.
14. Nikam PS, Mahale TR, Hasan M. J. Chem. Eng. Data. 1996; 41:1055.
15. Canosa J, Rodriguez A, Tojo J. J Chem.Eng. Data. 1998; 43:417.
16. Ortega J, Espiau F, Postigo M. J. Chem. Eng. Data. 2003; 48:916.
17. Ortega J, Espiau F, Postigo M. J Chem. Eng. Data.2004; 49:1602.
18. Ortega J, Espiau F, Postigo M. J Chem. Eng. Data.2005; 50:444.
19. B. Gonzalez, A. Dominguez, Jose Tojo, R. Cores, J. Chem. Eng. Data 49, 1225 (2004).
20. J. Wu, Z. Xu, Z. Liu, B. Wang, J. Chem. Eng. Data 50, 966 (2005).
21. U.B. Kadam, A.P. Hiray, A.B. Sawant, M. Hassan, J. Chem. Eng. Data 51, 60 (2006).
22. Joseph Kestin, Mordechai Sokolov, Willium A. Wakeham. J. Phys. Chem. Ref. Data, 1978, 7, 941-948.
23. Instruction manuals for ultrasonic interferometer model F-05, Constant temperature water bath Mittal Enterprises.
24. American Society for Testing and Materials (ASTM) Standard D6751. ASTM: West Conshohocken, PA, 2009.
25. Maurya.V.N, DiwinderKaurArora, Avadhesh Kumar Maurya Er , Gautam. R. A. World of Sciences Journal, 2013, 2, 27-50.
26. R. Palani, S. Saravanan, and R. Kumar, RasayanJ.Chem, 2009, 3, 622, 629.
27. T. Sumathi, and J Uma Maheswari, Indian Journal of Pure and Applied Physics, November, 2009, 782, 786.
28. H.F. Smith, A.S. Rosenberg, J. Chem. Soc. Part, 1963, 5391. N. V. Sastry and S. R. Patel, Int. J. Thermophys. 21, 1153 (2000).
29. M. V. Rathnam, S. M. K. Jain, and M. S. S. Kumar, J. Solution Chem. 41, 475 (2012).

30. G. Nath and R. Paikaray, Ind. J. Phys. 83, 1309 (2009).
31. D. S Wankhede, N. N. Wankhede, M. K. Lande, and B. R. Arbad, Ind. J. Pure Appl. Phys. 44, 909 (2006).
32. Vyas A D, Rana V A, Bhatnagar S P, Vashisth V M, Indian J. Pure and Appl. Phys. 46, 521 (2008).
33. Patil S P, Chaudari A S, Lokhande M P, Landle M K, Mehrotra S C, J. Chem. Eng. Data., 44, 875 (1999).
34. Madhu mohan T, Sreeharisastry S, Murthy V R K, Indian J. Pure Appl. Phys. 48, 668 (2010).
35. Sk.Suriyashihab, Shaik.Babu, S.Sreeharisastry, Rasayan J. Chem.,. 9(4), 641 (2016).
36. Sk.Suriyashihab, K.Govinda rao, M.Gnanakiran, Shaik.Babu, S.Sreeharisastry, Rasayan J. Chem10(1), 59 (2017).
37. A. Anis Fathima, M. Umadevi and V. Ramakrishnan. J. Raman Spectrosc, 2007, 38, 271, 276.
38. A. Anis Fathima, M. Umadevi, M. S. Ramachandran and V. Ramakrishnan. J. Raman Spectrosc, 2008, 38, 1639, 1645.
39. A.Anis Fathima, M. Umadevi and V. Ramakrishnan.J. Fluores, 2008, 18, 383, 391.
40. PT Ndifon, MO Agwara, NJ Njapba, MD Yufanyi, GA Paboudam and LD Nyamen, Research Journal of Chemistry and Environment, 2010, 2, 14, 50, 54.