Supplementary Information

Evaluation of molecular interactions between *o*-methoxy nitrobenzene and certain alcohols in *n*-hexane medium using ultrasonic sound at 303K

P S Syed Ibrahim*[a], J Edward Jeyakumar[b], N Venkatesh Kumar[a], E Rajasekaran[a] & Y Geetha[c]

[a] Department of Chemistry, VSB Engineering College, Karur 639 111, Tamil Nadu, India

[b] Department of Chemistry, DMI College of Engineering, Chennai 600 123, India

[c] Department of Chemistry, Chennai Institute of Technology, Chennai 600 069, India

E-mail: syedibuji@gmail.com

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Table S1- Procurement details

Name of the Chemicals	CAS-Number	Make	Purity mass fraction
o-methoxy nitro benzene	91-23-6	Sigma-Aldrich	99.0%
1-Propanol	71-23-8	Merck	99.7%
1-Butanol	71-36-3	Merck	99.8%
1-Pentanol	71-41-0	Merck	99.0%
n-Hexane	110-54-3	Sigma-Aldrich	95.0%

Table S2: Experimental values of ultrasonic velocity, density and viscosity for o-MNB+1-PRO/1-BUT/1-PEN in n-hexane medium at 303K.

Con.	Velocity (ms^{-1})			Density Kg/m^3			Viscosity$\times10^{-04}$ Nsm^{-2}		
10^{-03}M	1-PRO	1-BUT	1-PEN	1-PRO	1-BUT	1-PEN	1-PRO	1-BUT	1-PEN
1	1056.3	1035.8	1037.1	802.0	796.0	796.0	5.294	4.821	4.795
2	1058.0	1036.8	1037.5	802.0	796.0	796.0	5.021	4.442	4.548
3	1060.3	1037.7	1038.0	802.0	796.0	796.0	5.030	4.446	4.532
4	1062.5	1037.8	1038.2	802.0	796.0	796.0	5.073	4.454	4.573
5	1065.5	1037.8	1038.2	808.0	796.0	796.0	5.234	4.475	4.521
6	1067.0	1037.9	1038.7	808.0	797.0	796.0	5.247	4.517	4.502
7	1067.8	1038.9	1039.1	808.0	801.0	796.0	5.237	4.484	4.548
8	1068.0	1039.1	1039.5	808.0	801.0	796.0	5.296	4.485	4.588
9	1069.0	1040.3	1040.2	808.0	802.0	796.0	5.302	4.524	4.600
10	1070.4	1041.5	1040.7	809.0	803.0	797.0	5.371	4.534	4.638

Table S3: Calculated adiabatic compressibility (κ), acoustic impedance (Z), free length (L_f), and free volume (V_f) values for o-MNB+1-PRO/1-BUT/1-PEN in n-hexane medium at 303K.

Con. 10^{-03} M	(κ) $\times10^{-09}$ Kg^{-1} ms^2			(Z)$\times10^{05}$ $Kgm^{-2}s^{-1}$			(L_f)pm $\times10^{-11}$			(V_f) $\times10^{-07}$ m^3		
	1-PRO	1-BUT	1-PEN	1-PRO	1-BUT	1-PEN	1-PRO	1-BUT	1-PEN	1-PRO	1-BUT	1-PEN
1	1.13	1.17	1.18	8.40	8.25	8.19	6.66	6.79	6.81	3.274	3.658	3.005
2	1.12	1.15	1.17	8.48	8.27	8.20	6.57	6.73	6.79	2.667	3.108	3.022
3	1.11	1.14	1.15	8.50	8.29	8.24	6.55	6.72	6.78	2.669	3.109	3.083
4	1.10	1.13	1.14	8.52	8.30	8.26	6.54	6.70	6.76	2.643	3.101	3.023
5	1.09	1.11	1.13	8.61	8.32	8.27	6.50	6.68	6.72	2.532	3.079	3.053
6	1.08	1.10	1.11	8.62	8.34	8.29	6.49	6.65	6.71	2.528	3.039	3.011
7	1.06	1.09	1.10	8.63	8.35	8.30	6.48	6.64	6.70	2.539	3.035	2.974
8	1.04	1.06	1.08	8.63	8.36	8.31	6.46	6.62	6.69	2.497	3.032	2.965
9	1.02	1.05	1.06	8.64	8.37	8.32	6.44	6.61	6.68	2.496	3.030	2.931
10	1.01	1.03	1.04	8.66	8.39	8.33	6.43	6.59	6.64	2.452	3.022	2.452

Table S4: Calculated internal pressure ($\prod_i$), Lennard-Jones potential (LJP), available volume (V_a), and molar cohesive energy (MCE) and molecular interaction parameter (χ_u) values for o-MNB+1-PRO/1-BUT/1-PEN in n-hexane medium at 303K.

Con. 10^{-03} M	($\prod_i$) atm			LJP			(V_a) $\times10^{-05}m^3$			(MCE) KJ/mole			(χ_u)$\times10^{-01}$		
	1-pro	1-but	1-pen	1-pro	1-but	1-pen	1-pro	1-but	1-pen	1-pro	1-but	1-pen	1-pro	1-but	1-pen
1	2865	2747	2738	3.734	4.014	4.052	4.356	4.514	4.504	36.98	41.41	39.22	-2.649	-2.932	-2.913
2	3485	3295	3317	4.711	4.040	4.063	3.555	3.722	3.717	37.04	41.31	39.28	-2.626	-2.918	-2.908
3	3488	3295	3322	4.786	4.070	4.079	3.540	3.716	3.714	37.04	41.58	39.32	-2.594	-2.906	-2.902
4	3496	3298	3333	4.856	4.075	4.088	3.526	3.715	3.712	37.15	41.55	39.37	-2.563	-2.905	-2.899
5	3549	3305	3344	5.873	4.073	4.087	3.480	3.715	3.712	37.55	42.38	39.12	-2.521	-2.905	-2.899
6	3554	3310	3348	4.958	4.076	4.102	3.470	3.710	3.709	37.63	42.49	38.85	-2.500	-2.904	-2.892
7	3555	3320	3350	5.009	4.111	4.116	3.463	3.684	3.709	37.78	41.69	38.98	-2.489	-2.890	-2.887

				5.0	4.11										
8	3577	3324	3355	46	5	4.129	3.463	3.683	3.706	37.79	42.07	39.26	-2.486	-2.888	-2.881
				5.0	4.14										
9	3581	3339	3358	66	9	4.147	3.456	3671	3.699	37.80	42.10	39.39	-2.473	-2.871	-2.873
				5.1	4.16										
10	3602	3341	3361	28	2	4.161	3.443	3.663	3.691	38.15	43.31	39.54	-2.453	-2.855	-2.866

Table S5- Excess adiabatic compressibility, excess free length and excess ultrasonic velocity of o-MNB+1-PRO/1-BUT/1-PEN in n-hexane medium at 303K.

	Excess adiabatic compressibility$\times10^{-10}$ $Kg^{1}ms^{2}$			Excess free length$\times10^{-10}$ m			Excess ultrasonic velocity (m/s)		
Con.$\times10^{-3}$ M	1-pro	1-but	1-pen	1-pro	1-but	1-pen	1-pro	1-but	1-pen
1	-4.53	-3.21	-3.12	-7.19	-7.02	-6.99	-33.05	-52.65	-62.06
2	-7.97	-4.69	-4.67	-7.52	-7.20	-7.15	-45.60	-84.05	-85.38
3	-11.55	-6.31	-6.29	-7.83	-7.37	-7.29	-56.97	-113.98	-117.73
4	-15.64	-8.11	-8.09	-8.11	-7.53	-7.42	-67.60	-143.47	-149.47
5	-20.10	-10.21	-10.09	-8.38	-7.70	-7.55	-77.52	-171.64	-180.51
6	-25.12	-12.45	-12.33	-8.63	-7.85	-7.67	-87.06	-198.62	-210.66
7	-30.82	-14.98	-14.95	-8.86	-8.01	-7.79	-96.01	-223.53	-239.41
8	-37.35	-17.85	-17.82	-9.08	-8.16	-7.91	-104.36	-248.28	-267.70
9	-44.99	-21.25	-21.22	-9.29	-8.30	-8.02	-112.21	-270.98	-295.08
10	-54.41	-24.96	-24.03	-9.59	-8.44	-8.12	-119.63	-292.68	-321.89

Table S6: Excess free volume, excess internal pressure and excess acoustic impedance of o-MNB+1-PRO/1-BUT/1-PEN in n-hexane medium at 303K.

	Excess free volume$\times10^{-7}$ m^3			Excess Internal Pressure$\times10^{8}$ Nm^{-2}			Excess Acoustic Impedance$\times10^{5}Kgs^{-1}$		
Con.$\times10^{-3}$ M	1-pro	1-but	1-pen	1-pro	1-but	1-pen	1-pro	1-but	1-pen
1	1.063	6.4	10.27	-1.54	-1.53	-1.44	1.50	1.48	1.47
2	0.979	6.4	10.83	-2.06	-2.06	-1.87	1.68	1.6	1.53
3	0.955	6.0	10.42	-2.26	-2.26	-1.99	1.80	1.7	1.60
4	0.932	5.9	10.50	-2.42	-2.38	-2.11	1.92	1.8	1.65
5	0.973	4.8	10.30	-2.62	-2.41	-2.23	2.04	1.9	1.71
6	0.969	4.4	10.53	-2.79	-2.56	-2.35	2.16	2.0	1.76
7	0.991	5.1	10.55	-2.94	-2.66	-2.46	2.27	2.1	1.82
8	0.981	5.0	10.83	-3.08	-2.88	-2.56	2.38	2.3	1.82
9	0.900	4.3	9.75	-3.24	-2.87	-2.67	2.51	2.4	1.97
10	0.866	3.8	9.75	-3.32	-3.05	-2.77	2.42	2.6	2.02

Table S7- Formation constant (K), free energy change (ΔG_F), enthalpy change (ΔH), entropy change (ΔS) and viscous relaxation time (τ) for the formation of hydrogen bonded complex betweeno-MNB+1-PRO/1-BUT/1-PEN in n-hexane medium at 303K.

H-Acceptor: o-MNB

H-Donor	K/ M^{-1}	ΔG_F /kJ mol^{-1}	ΔH/ /kJ mol^{-1}	ΔS/J K^{-1} mol^{-1}	Relaxation time τ/ fs
1-Propanol	18.8	-8.10	-31.4	-86	6.8
1-Butanol	17.3	-7.3	-25.2	-59	6.8
1-Pentanol	13.6	-6.95	-21.2	-47	6.9

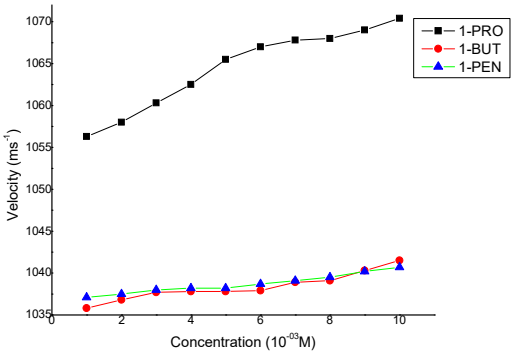

Fig. S1 Plot of ultrasonic velocity against molar concentration

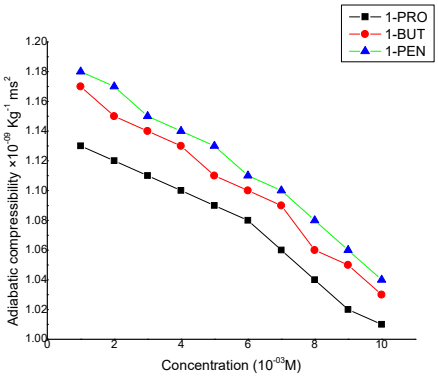

Fig. S2 Plot of adiabatic compressibility against molar concentration

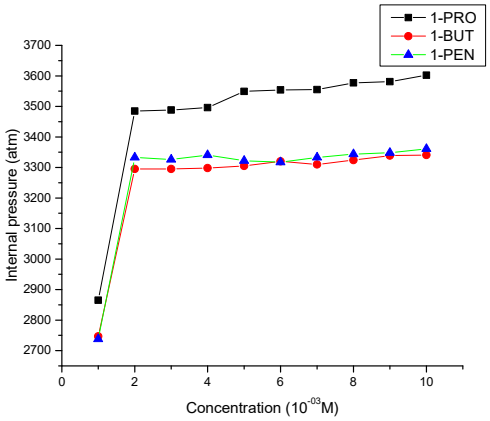

Fig. S3 Plot of internal pressure against molar concentration

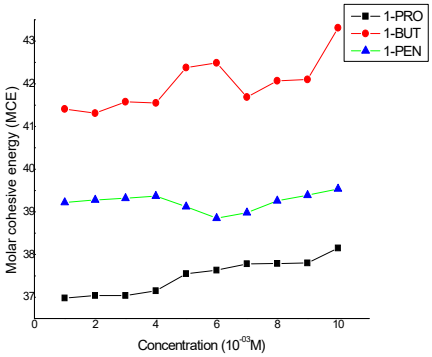

Fig. S4 Plot of molar cohesive energy against molar concentration

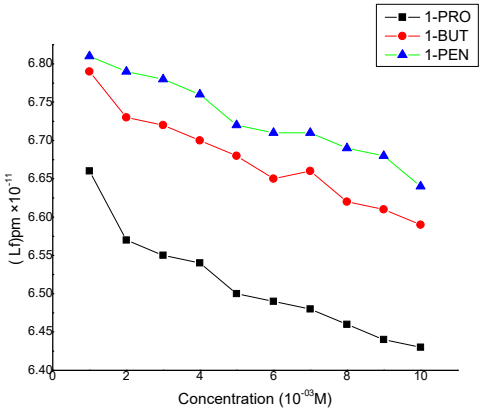

Fig. S5 Plot of free length against molar concentration.

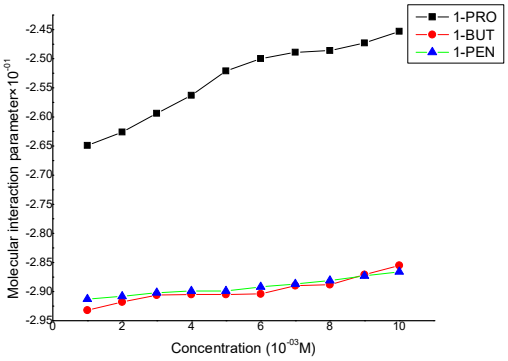

Fig. S6 Plot of molecular interaction parameter against molar concentration.

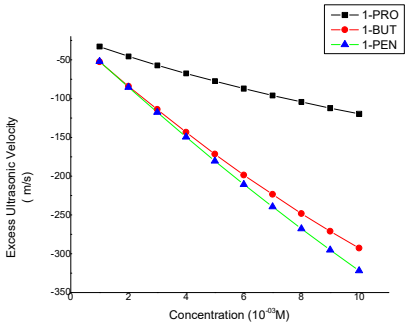

Fig. S7 Plot of excess ultrasonic velocity vs concentration

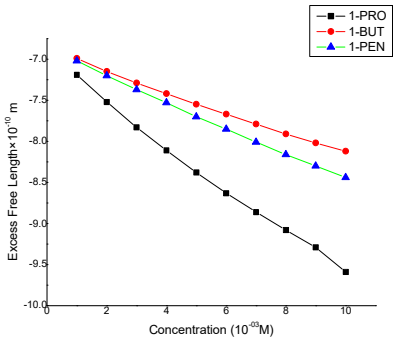

Fig. S10 Plot of excess free length vs concentration

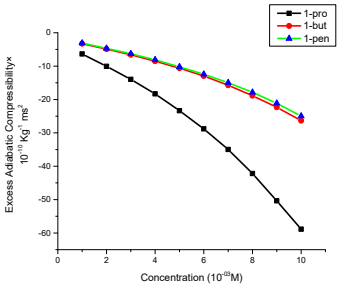

Fig. S8 Plot of Excess adiabatic compressibility vs Concentration

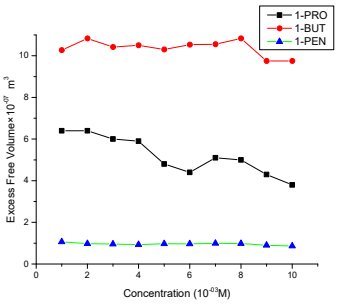

Fig. S11 Plot of excess free volume vs Concentration

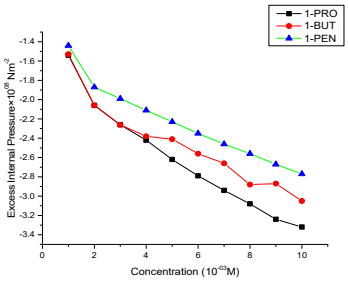

Fig. S9 Plot of excess internal pressure vs concentration

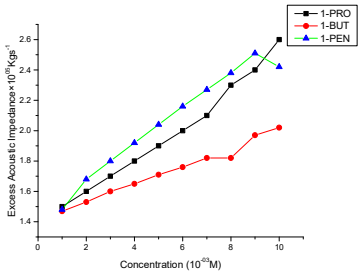

Fig. S12 Plots of excess acoustic impedance vs concentration