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DFT Study, Volume Changes with Molecular Interactions of Hydroquinone in Water, Alcohol and Binary Solvent Mixtures of Aqueous Alcohol at Different Temperatures

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ABSTRACT

Densities of water, ethanol, 1-propanol and binary solvent mixture of water+ethanol, water+1-propanol were experimentally measured. Experimental density data used to calculate the excess molar volumes (V^E). Redlich−Kister Equation was used to calculate excess molar volumes (V^E) to correlate with the experimental excess molar volumes (V^E) of binary solvent mixture. Regressed Parameters Ai obtained from Redlich−Kister Equation were used for calculation of partial excess molar volumes at infinite dilution ($\overline{V}_i^{E,\infty}$). In these same solvents hydroquinone was added to make saturated solutions of hydroquinone at equilibrium. These saturated supernatant solutions were used to measured densities and molalities of hydroquinone at (293.15 to 313.15) K and apparent molar volume (V_Φ). Molecular interaction was explain by using Gaussian 09W software, DFT method, B3LYP 6-31(G)d as basis set.

KEYWORD: *DFT, Hydroquinone, Excess Molar Volumes (V^E), Apparent Molar Volume (V_Φ).*

INTRODUCTION

Hydroquinone, the major benzene metabolite, is a ubiquitous chemical in the environment due to its widespread application in human and industrial activities. It can be used as a developing agent in photography, dye intermediate, stabilizer in paints, varnishes oils and motor fuels. In addition, hydroquinone has been used as an antioxidant in the rubber and food industry. From 1950s to 2001 hydroquinone was applied in the commercially available cosmetic skin lightening formulations in European Union countries and since 1960s it was commercially available as a medical product. It is also present in cosmetic formulations of products for coating finger nails and hair dyes [1, 2]. The antimicrobial properties of arbutin as the main compound and hydroquinone as the active metabolite were determined and compared with the antimicrobial properties of *A. unedo leaf* extracts so as to test the extent to which arbutin is responsible for antimicrobial activity [3]. Hydroquinone is crystalline white solid. IUPAC name is benzene-1, 4-diol with the molecular formula $C_6H_6O_2$. Molar mass is 110.11 gm/mol, melting point is about 172^0C.

DFT is very popular in the field of chemistry for interpretation of structure and reactivity of various organic molecules. Theoretical data obtained by Gaussian 09W software is very good agreement

with the instrumental analysis of organic molecules [4, 5]. Here we used DFT to explaining interaction between solvent-solvent and solute-solvent molecules. Solvent-solvent and solvent-solute interactions of electrolytes are extremely important for the synthesis, design of processes and simulations of unit operations [6]. Densities of pure water, alcohols at certain temperatures were available but in water+alcohol mixed solvent system for 0.1 to 0.9 mole fractions of ethanol and 1-propanol have to be investigating. We have undertaken the measurements of densities of pure solvents, binary solvent mixtures and saturated solutions of hydroquinone in water + methanol and water+1-propanol binary solvents over the entire composition range from 0 to 1 mole fraction of ethanol and 1-propanol. The experimental work was carried out at (293.15 to 313.15) K and excess molar volumes (V^E) [7] were calculated from the measured densities of the pure components and the binary mixtures as shown in Table 1 & 2.

Table 1-Mole fraction of methanol (x^0_C), density ρ, experimental [$V^E_{(Exp.)}$] & calculated [$V^E_{(Cal.)}$] values of excess molar volumes of water + ethanol binary system and molality (m), density (ρ), apparent molar volume (V_Φ) of Hydroquinone + water + ethanol ternary system at temperatures (293.15 to 313.15) K & pressure 101.32 kPa^a.

x^0_C	Binary solvent $\rho.10^{-3}$ /kg.m^{-3}	$V^E_{(Exp.)}$ 10^6.m^3.mol^{-1}	$V^E_{(Cal.)}$ 10^6.m^3.mol^{-1}	m mol.Kg^{-1}	Ternary solution $\rho.10^{-3}$/ kg.m^{-3}	V_Φ m^3.mol^{-1}
			293.15 K			
0.0000	0.9982	0.0000	0.0000	0.5708	1.0090	90.3332
0.1008	0.9659	-0.5237	-0.5280	1.7598	0.9992	90.5514
0.2000	0.9374	-0.8907	-0.8719	3.1990	0.9980	90.0969
0.3001	0.9094	-1.0529	-1.0548	4.2185	0.9941	88.5434
0.3999	0.8844	-1.0804	-1.1117	4.8867	0.9875	87.3346
0.5000	0.8639	-1.0741	-1.0835	5.2260	0.9795	86.2941
0.5999	0.8468	-1.0340	-0.9964	5.3653	0.9698	85.6175
0.7002	0.8304	-0.8648	-0.8550	5.4262	0.9598	84.8004
0.8000	0.8156	-0.6250	-0.6493	5.3807	0.9489	84.0051
0.8999	0.8029	-0.3684	-0.3634	5.1909	0.9379	82.8687
1.0000	0.7905	0.0000	0.0000	5.0169	0.9259	82.0370
			295.65 K			
0.0000	0.9977	0.0000	0.0000	0.6306	1.0097	90.1553
0.1008	0.9646	-0.5214	-0.5255	1.9315	1.0009	90.5824
0.2000	0.9355	-0.8807	-0.8633	3.4063	1.0001	89.8481
0.3001	0.9073	-1.0428	-1.0438	4.4167	0.9950	88.6548
0.3999	0.8823	-1.0745	-1.1029	5.0253	0.9882	87.2584
0.5000	0.8616	-1.0646	-1.0793	5.4003	0.9795	86.5406
0.5999	0.8447	-1.0382	-0.9966	5.5691	0.9702	86.0140
0.7002	0.8281	-0.8648	-0.8574	5.5836	0.9602	84.9258
0.8000	0.8134	-0.6282	-0.6514	5.5317	0.9491	84.2240
0.8999	0.8006	-0.3688	-0.3640	5.3197	0.9381	82.9636
1.0000	0.7882	0.0000	0.0000	5.1587	0.9268	82.0470

			298.15 K			
0.0000	0.9970	0.0000	0.0000	0.6870	1.0102	90.0098
0.1008	0.9634	-0.5196	-0.5231	2.0967	1.0024	90.5927
0.2000	0.9337	-0.8723	-0.8575	3.6102	1.0014	89.9172
0.3001	0.9053	-1.0345	-1.0350	4.6062	0.9961	88.6922
0.3999	0.8803	-1.0685	-1.0932	5.2115	0.9892	87.3122
0.5000	0.8595	-1.0582	-1.0715	5.5835	0.9805	86.5870
0.5999	0.8426	-1.0317	-0.9923	5.7572	0.9707	86.2327
0.7002	0.8259	-0.8578	-0.8563	5.7317	0.9606	85.0238
0.8000	0.8114	-0.6333	-0.6509	5.6267	0.9494	84.1383
0.8999	0.7984	-0.3657	-0.3619	5.4343	0.9384	82.9802
1.0000	0.7861	0.0000	0.0000	5.3044	0.9271	82.3085
			300.65 K			
0.0000	0.9964	0.0000	0.0000	0.7541	1.0108	89.9946
0.1008	0.9619	-0.5159	-0.5197	2.3021	1.0041	90.6717
0.2000	0.9317	-0.8615	-0.8454	3.8280	1.0024	90.0679
0.3001	0.9030	-1.0200	-1.0206	4.8430	0.9974	88.7357
0.3999	0.8778	-1.0553	-1.0818	5.4301	0.9900	87.4681
0.5000	0.8571	-1.0484	-1.0629	5.7915	0.9815	86.6572
0.5999	0.8402	-1.0240	-0.9837	5.8839	0.9713	86.0560
0.7002	0.8235	-0.8520	-0.8463	5.9103	0.9608	85.2386
0.8000	0.8088	-0.6217	-0.6429	5.8299	0.9501	84.3484
0.8999	0.7961	-0.3652	-0.3608	5.5779	0.9384	83.1860
1.0000	0.7837	0.0000	0.0000	5.4030	0.9271	82.2409
			303.15 K			
0.0000	0.9957	0.0000	0.0000	0.8304	1.0113	90.1249
0.1008	0.9605	-0.5143	-0.5175	2.5057	1.0065	90.4157
0.2000	0.9297	-0.8533	-0.8400	4.1095	1.0046	90.0783
0.3001	0.9009	-1.0146	-1.0130	5.0990	0.9990	88.8337
0.3999	0.8756	-1.0493	-1.0742	5.6852	0.9910	87.7222
0.5000	0.8548	-1.0441	-1.0579	6.0105	0.9819	86.9437
0.5999	0.8378	-1.0211	-0.9821	6.1101	0.9720	86.3234
0.7002	0.8211	-0.8478	-0.8464	6.0841	0.9615	85.2933
0.8000	0.8065	-0.6241	-0.6412	5.9599	0.9502	84.4098
0.8999	0.7936	-0.3598	-0.3561	5.7400	0.9391	83.2605
1.0000	0.7813	0.0000	0.0000	5.5413	0.9279	82.1824
			305.65 K			
0.0000	0.9949	0.0000	0.0000	0.9084	1.0119	90.2538
0.1008	0.9592	-0.5118	-0.5149	2.7181	1.0081	90.6113
0.2000	0.9278	-0.8434	-0.8306	4.3552	1.0063	90.0959
0.3001	0.8988	-1.0039	-1.0017	5.3480	1.0004	88.9328
0.3999	0.8735	-1.0399	-1.0646	5.9113	0.9921	87.8300
0.5000	0.8526	-1.0348	-1.0497	6.2289	0.9827	87.1288
0.5999	0.8357	-1.0139	-0.9733	6.4306	0.9728	86.9679
0.7002	0.8189	-0.8376	-0.8374	6.3440	0.9619	85.8476

0.8000	0.8043	-0.6193	-0.6359	6.1520	0.9508	84.6707
0.8999	0.7915	-0.3618	-0.3582	5.8882	0.9396	83.3790
1.0000	0.7792	0.0000	0.0000	5.6422	0.9280	82.1754
			308.15 K			
0.0000	0.9940	0.0000	0.0000	1.0176	1.0127	90.5091
0.1008	0.9578	-0.5115	-0.5145	2.9533	1.0099	90.7748
0.2000	0.9259	-0.8373	-0.8245	4.6569	1.0083	90.2254
0.3001	0.8967	-0.9961	-0.9946	5.6107	1.0016	89.1070
0.3999	0.8714	-1.0362	-1.0598	6.1314	0.9934	87.8679
0.5000	0.8505	-1.0321	-1.0463	6.3811	0.9838	86.9639
0.5999	0.8334	-1.0067	-0.9686	6.6669	0.9732	87.2792
0.7002	0.8167	-0.8326	-0.8310	6.3822	0.9624	85.3508
0.8000	0.8021	-0.6154	-0.6321	6.3181	0.9514	84.7870
0.8999	0.7894	-0.3647	-0.3611	6.0356	0.9398	83.5797
1.0000	0.7771	0.0000	0.0000	5.8023	0.9286	82.3755
			310.65 K			
0.0000	0.9932	0.0000	0.0000	1.1278	1.0135	90.7187
0.1008	0.9563	-0.5093	-0.5120	3.2094	1.0123	90.7581
0.2000	0.9240	-0.8325	-0.8215	4.8698	1.0098	90.1574
0.3001	0.8946	-0.9890	-0.9895	5.8501	1.0029	89.1654
0.3999	0.8696	-1.0404	-1.0522	6.3664	0.9943	88.0807
0.5000	0.8481	-1.0130	-1.0376	6.6237	0.9845	87.1719
0.5999	0.8311	-0.9973	-0.9606	6.8092	0.9743	87.0553
0.7002	0.8145	-0.8308	-0.8239	6.5730	0.9632	85.4805
0.8000	0.7998	-0.6056	-0.6242	6.4598	0.9525	84.5740
0.8999	0.7871	-0.3558	-0.3520	6.1785	0.9408	83.4685
1.0000	0.7749	0.0000	0.0000	5.9648	0.9295	82.4776
			313.15 K			
0.0000	0.9922	0.0000	0.0000	1.2823	1.0146	91.1803
0.1008	0.9548	-0.5055	-0.5084	3.4963	1.0148	90.7890
0.2000	0.9218	-0.8180	-0.8050	5.2033	1.0119	90.2401
0.3001	0.8923	-0.9737	-0.9768	6.1273	1.0045	89.1797
0.3999	0.8675	-1.0392	-1.0544	6.6474	0.9957	88.2720
0.5000	0.8464	-1.0316	-1.0510	6.8638	0.9856	87.3952
0.5999	0.8293	-1.0162	-0.9727	7.0583	0.9754	87.3097
0.7002	0.8121	-0.8180	-0.8253	6.8208	0.9641	85.7340
0.8000	0.7976	-0.6061	-0.6174	6.7710	0.9532	85.3015
0.8999	0.7849	-0.3521	-0.3493	6.3960	0.9419	83.6792
1.0000	0.7727	0.0000	0.0000	6.1425	0.9302	82.6999

[a]Standard uncertainties u are u(T) = 0.01 K, u(x^0_C) = 0.0001, $u(p)$ = 0.01 MPa, $u(m)$ = 2×10^{-5} mol·kg^{-1} and the combined expanded uncertainties $U_c(\rho)$ = 0.00005 10^{-3}kg·m^{-3}, $U_c(V_\Phi)$ = 0.001 10^6.m^3·mol^{-1} and $U_c(V^E)$ = 0.001 10^6.m^3·mol^{-1}

Table 2- Mole fraction of 1-propanol (x^0_C), density ρ, experimental [$V^E_{(Exp.)}$] & calculated [$V^E_{(Cal.)}$] values of excess molar volumes of water + 1-Propanol binary system and molality (m), density (ρ), apparent molar volume (V_Φ) of Hydroquinone + water + 1-propanol ternary system at temperatures (293.15 to 313.15) K & pressure 101.32 kPa^a.

x^0_C	Binary solvent $\rho.10^{-3}$ /kg.m^{-3}	$V^E_{(Exp.)}$ 10^6.m^3.mol^{-1}	$V^E_{(Cal.)}$ 10^6.m^3.mol^{-1}	m mol.Kg^{-1}	Ternary solution $\rho.10^{-3}$/ kg.m^{-3}	V_Φ m^3.mol^{-1}
			293.15 K			
0.0000	0.9982	0.0000	0.0000	0.5708	1.0090	90.3332
0.1000	0.9551	-0.4564	-0.4544	2.4256	1.0037	88.7920
0.2001	0.9180	-0.6101	-0.6222	3.6010	0.9955	87.0493
0.3000	0.8913	-0.7010	-0.6814	4.2062	0.9850	86.4121
0.3999	0.8697	-0.6893	-0.7015	4.4813	0.9737	85.6774
0.4995	0.8541	-0.7037	-0.6958	4.4987	0.9625	85.0997
0.6002	0.8407	-0.6513	-0.6574	4.4218	0.9511	84.5538
0.7001	0.8297	-0.5744	-0.5805	4.2728	0.9393	84.3057
0.7926	0.8209	-0.4670	-0.4721	4.0624	0.9287	83.7389
0.8930	0.8120	-0.2828	-0.3015	3.7604	0.9159	83.0619
1.0000	0.8032	0.0000	0.0000	3.4142	0.9018	82.2382
			295.65 K			
0.0000	0.9977	0.0000	0.0000	0.6306	1.0097	90.1553
0.1000	0.9535	-0.4457	-0.4442	2.5195	1.0043	88.5758
0.2001	0.9161	-0.5983	-0.6076	3.7625	0.9959	87.3227
0.3000	0.8892	-0.6902	-0.6727	4.4261	0.9853	86.9975
0.3999	0.8676	-0.6765	-0.7034	4.6276	0.9742	85.7830
0.4995	0.8529	-0.7449	-0.7048	4.6912	0.9630	85.7762
0.6002	0.8385	-0.6391	-0.6646	4.5570	0.9513	84.6956
0.7001	0.8276	-0.5692	-0.5773	4.3834	0.9395	84.3636
0.7926	0.8188	-0.4704	-0.4575	4.1727	0.9288	83.8776
0.8930	0.8099	-0.2808	-0.2831	3.8551	0.9159	83.1401
1.0000	0.8011	0.0000	0.0000	3.5395	0.9025	82.3550
			298.15 K			
0.0000	0.9970	0.0000	0.0000	0.6870	1.0102	90.0098
0.1000	0.9519	-0.4356	-0.4361	2.6944	1.0057	88.6294
0.2001	0.9144	-0.5903	-0.5912	3.9419	0.9972	87.3735
0.3000	0.8872	-0.6770	-0.6597	4.6130	0.9866	86.9884
0.3999	0.8655	-0.6625	-0.6978	4.8473	0.9747	86.2662
0.4995	0.8507	-0.7234	-0.7001	4.8146	0.9635	85.6813
0.6002	0.8366	-0.6414	-0.6512	4.6758	0.9517	84.7742
0.7001	0.8256	-0.5684	-0.5528	4.4911	0.9398	84.3894
0.7926	0.8162	-0.4196	-0.4313	4.2655	0.9289	83.6739

0.8930	0.8078	-0.2726	-0.2707	3.9633	0.9159	83.3375
1.0000	0.7991	0.0000	0.0000	3.6298	0.9029	82.3035
			300.65 K			
0.0000	0.9964	0.0000	0.0000	0.7541	1.0108	89.9946
0.1000	0.9502	-0.4263	-0.4265	2.8836	1.0071	88.7129
0.2001	0.9123	-0.5770	-0.5816	4.1358	0.9982	87.4977
0.3000	0.8851	-0.6652	-0.6431	4.7693	0.9873	86.9944
0.3999	0.8633	-0.6505	-0.6689	5.0039	0.9757	86.1966
0.4995	0.8471	-0.6430	-0.6620	4.9996	0.9642	85.5231
0.6002	0.8343	-0.6279	-0.6138	4.8445	0.9520	85.0657
0.7001	0.8232	-0.5522	-0.5263	4.6347	0.9400	84.5673
0.7926	0.8136	-0.3948	-0.4186	4.3716	0.9291	83.5796
0.8930	0.8055	-0.2728	-0.2689	4.0560	0.9160	83.2997
1.0000	0.7968	0.0000	0.0000	3.7292	0.9030	82.3451
			303.15 K			
0.0000	0.9957	0.0000	0.0000	0.8304	1.0113	90.1249
0.1000	0.9484	-0.4151	-0.4145	3.1069	1.0088	88.8236
0.2001	0.9103	-0.5666	-0.5745	4.3696	0.9997	87.6649
0.3000	0.8830	-0.6545	-0.6330	4.9502	0.9888	86.8532
0.3999	0.8611	-0.6399	-0.6521	5.1819	0.9768	86.1790
0.4995	0.8448	-0.6272	-0.6447	5.1797	0.9647	85.7096
0.6002	0.8320	-0.6181	-0.6054	5.0081	0.9524	85.2593
0.7001	0.8209	-0.5427	-0.5286	4.7874	0.9403	84.7673
0.7926	0.8116	-0.4084	-0.4220	4.4957	0.9292	83.8111
0.8930	0.8032	-0.2630	-0.2608	4.1665	0.9162	83.3124
1.0000	0.7946	0.0000	0.0000	3.8312	0.9032	82.3853
			305.65 K			
0.0000	0.9949	0.0000	0.0000	0.9084	1.0119	90.2538
0.1000	0.9468	-0.4072	-0.4072	3.2781	1.0106	88.6206
0.2001	0.9086	-0.5625	-0.5671	4.6443	1.0019	87.8338
0.3000	0.8810	-0.6462	-0.6261	5.1720	0.9897	87.1512
0.3999	0.8590	-0.6272	-0.6440	5.3651	0.9778	86.2257
0.4995	0.8427	-0.6174	-0.6345	5.3207	0.9655	85.6525
0.6002	0.8299	-0.6123	-0.5942	5.1832	0.9531	85.4940
0.7001	0.8187	-0.5335	-0.5197	4.8968	0.9405	84.7734
0.7926	0.8095	-0.4022	-0.4183	4.6013	0.9294	83.8293
0.8930	0.8012	-0.2661	-0.2633	4.2905	0.9166	83.5131
1.0000	0.7925	0.0000	0.0000	3.9392	0.9036	82.4557
			308.15 K			
0.0000	0.9940	0.0000	0.0000	1.0176	1.0127	90.5091
0.1000	0.9452	-0.4011	-0.4020	3.5409	1.0125	88.8971

0.2001	0.9066	-0.5494	-0.5483	4.8604	1.0029	88.0143
0.3000	0.8790	-0.6351	-0.6175	5.3881	0.9909	87.2879
0.3999	0.8570	-0.6168	-0.6569	5.5626	0.9785	86.4673
0.4995	0.8420	-0.6821	-0.6585	5.5534	0.9663	86.4510
0.6002	0.8279	-0.6037	-0.6088	5.3369	0.9536	85.6337
0.7001	0.8168	-0.5294	-0.5141	5.0734	0.9408	85.2076
0.7926	0.8074	-0.3890	-0.4028	4.7395	0.9296	84.0810
0.8930	0.7992	-0.2616	-0.2592	4.3904	0.9170	83.4443
1.0000	0.7905	0.0000	0.0000	4.0441	0.9037	82.6607
			310.65 K			
0.0000	0.9932	0.0000	0.0000	1.1278	1.0135	90.7187
0.1000	0.9436	-0.3956	-0.3968	3.7919	1.0139	89.2183
0.2001	0.9047	-0.5415	-0.5382	5.0778	1.0046	87.9747
0.3000	0.8770	-0.6287	-0.6135	5.6152	0.9922	87.4107
0.3999	0.8549	-0.6108	-0.6612	5.7602	0.9796	86.5702
0.4995	0.8405	-0.7098	-0.6634	5.7020	0.9668	86.6225
0.6002	0.8257	-0.5916	-0.6052	5.5067	0.9543	85.7312
0.7001	0.8144	-0.5046	-0.5010	5.2323	0.9411	85.3883
0.7926	0.8053	-0.3866	-0.3909	4.8911	0.9301	84.3189
0.8930	0.7971	-0.2626	-0.2616	4.5178	0.9175	83.5743
1.0000	0.7884	0.0000	0.0000	4.1665	0.9043	82.7677
			313.15 K			
0.0000	0.9922	0.0000	0.0000	1.2823	1.0146	91.1803
0.1000	0.9417	-0.3856	-0.3865	4.0812	1.0161	89.3168
0.2001	0.9025	-0.5259	-0.5274	5.3720	1.0064	88.0990
0.3000	0.8748	-0.6153	-0.5916	5.8945	0.9936	87.6203
0.3999	0.8526	-0.5987	-0.6272	6.0126	0.9806	86.8222
0.4995	0.8366	-0.6073	-0.6306	5.9483	0.9680	86.4649
0.6002	0.8241	-0.6323	-0.5910	5.7084	0.9550	86.1713
0.7001	0.8123	-0.5144	-0.5120	5.3672	0.9416	85.4478
0.7926	0.8032	-0.3976	-0.4144	5.0464	0.9308	84.4883
0.8930	0.7951	-0.2786	-0.2752	4.6553	0.9181	83.7322
1.0000	0.7862	0.0000	0.0000	4.2938	0.9052	82.7018

[a]Standard uncertainties u are u(T) = 0.01 K, u(x^0_C) = 0.0001, $u(p)$ = 0.01 MPa, $u(m) = 2\times10^{-5}$ mol·kg^{-1} and the combined expanded uncertainties $U_c(\rho) = 0.00005\ 10^{-3}$kg·m^{-3}, $U_c(V_\Phi) = 0.001\ 10^{6}$.m^{3}·mol^{-1} and $U_c(V^E) = 0.001\ 10^{6}$.m^{3}·mol^{-1}

Excess molar volume of binary mixture can be defined as the difference in molar volume of the mixture and the sum of the molar volume each component at given conditions [8]. The excess molar volumes (V^E) for the binary mixtures were obtained by eq.1.

$$V^E = [x_1 M_1 + x_2 M_2]/\rho_{12} - x_1 M_1/\rho_1 - x_2 M_2/\rho_2 \quad ....(1)$$

Where *xi*, *ρi,* and *Mi* represent the mole fraction, the density and the molecular weight of the pure component respectively, while ρ_{12} represents the density of the binary solvent mixtures.
The values of experimental V^E for water+methanol binary solvent mixture were compared with calculated values of V^E by Redlich−Kister [9] type smoothing equation:

$$V^E = x_1 x_2 \sum_{i=o}^{n} Ai(x_1 - x_2)^i \qquad \text{.....(2)}$$

Where x_1 was the molar fraction of alcohols used in study, x_2 was mole fraction of water, *Ai* was the adjustable parameter, and n was the number of the fitted parameters. The parameters for the Redlich−Kister equation was obtained by the least-squares fit method and the results were listed in Table 3.

Table 3- Regressed Parameters *Ai* and correlation coefficient R^2 of the Redlich−Kister Equation and the Root-Mean-Square Deviation (σ)

*T*K	A_0 $10^6.m^3{\cdot}mol^{-1}$	A_1 $10^6.m^3{\cdot}mol^{-1}$	A_2 $10^6.m^3{\cdot}mol^{-1}$	A_3 $10^6.m^3{\cdot}mol^{-1}$	A_4 $10^6.m^3{\cdot}mol^{-1}$	R^2	σ
Ethanol + Water							
293.15	-4.334056	1.208494	-1.470479	-0.136927	0.842451	0.976	0.020
295.65	-4.317362	1.109239	-1.435662	-0.015585	0.772472	0.975	0.020
298.15	-4.286136	1.049181	-1.496145	0.075723	0.852436	0.981	0.018
300.65	-4.251799	1.019337	-1.293966	0.098478	0.511602	0.977	0.019
303.15	-4.231778	0.952430	-1.319737	0.230746	0.596808	0.981	0.018
305.65	-4.198983	0.945459	-1.175141	0.190700	0.296780	0.980	0.018
308.15	-4.185171	0.946444	-1.008507	0.154689	-0.032831	0.981	0.017
310.65	-4.150586	0.947381	-1.070432	0.223437	0.136931	0.982	0.017
313.15	-4.204077	0.837268	-0.445638	0.387798	-0.625269	0.980	0.018
1-Propanol + Water							
293.15	-2.782921	0.410708	-1.155010	1.180108	-1.453315	0.995	0.012
295.65	-2.818734	0.348533	-0.720844	1.362090	-1.661118	0.984	0.020
298.15	-2.799907	0.433119	-0.180125	1.262211	-2.292545	0.988	0.017
300.65	-2.647679	0.531599	-0.543446	1.018761	-1.947570	0.985	0.017
303.15	-2.578455	0.440422	-0.992289	1.128049	-1.130985	0.991	0.013
305.65	-2.537695	0.479510	-1.010339	0.957434	-1.142175	0.989	0.014
308.15	-2.633524	0.461279	-0.002879	0.959783	-2.374472	0.983	0.018
310.65	-2.653254	0.553001	0.485876	0.722104	-3.066627	0.974	0.024
313.15	-2.522124	0.344036	-0.316517	0.804757	-2.157189	0.974	0.021

The values of the partial excess volume as given in Table-4 for solvent$_1$ and solvent$_2$ at infinite dilution $\overline{V_1}^{E,\infty}$ have been calculated from the adjustable parameters of Redlich−Kister smoothing equation as

$$\overline{V_1}^{E,\infty} = A_0 - A_1 + A_2 - A_3 + A_4 \qquad \text{... (3)}$$

$$\overline{V_2}^{E,\infty} = A_0 + A_1 + A_2 + A_3 + A_4 \qquad \text{.... (4)}$$

Table 4- Calculated Partial Excess Molar Volumes at Infinite Dilution at T = (293.15 to 313.15) K from Redlich−Kister Parameters *Ai*

	Ethanol(1) + Water(2)		1-Propanol(1) + Water(2)	
	$\bar{V}_1^{E,\infty}$	$\bar{V}_2^{E,\infty}$	$\bar{V}_1^{E,\infty}$	$\bar{V}_2^{E,\infty}$
T(K)	$10^6.m^3{\cdot}mol^{-1}$	$10^6.m^3{\cdot}mol^{-1}$	$10^6.m^3{\cdot}mol^{-1}$	$10^6.m^3{\cdot}mol^{-1}$
293.15	-6.033652	-3.890518	-6.982062	-3.800430
295.65	-6.074206	-3.886898	-6.911319	-3.490074
298.15	-6.054749	-3.804943	-6.967907	-3.577248
300.65	-6.151978	-3.916347	-6.689055	-3.588334
303.15	-6.137882	-3.771531	-6.270201	-3.133259
305.65	-6.213503	-3.941184	-6.127152	-3.253265
308.15	-6.327641	-4.125377	-6.431937	-3.589813
310.65	-6.254905	-3.913270	-6.509109	-3.958900
313.15	-6.500051	-4.049917	-6.144622	-3.847037

The following equation was used to calculate the root-mean-square deviation (rmsd) values:

$$rmsd(\sigma) = \sqrt{\frac{1}{N}\sum_i^N (V^E_{cal\,(i)} - V^E_{exp_{(i)}})^2} \quad \text{.... (5)}$$

Where $V^E_{cal(i)}$ and $V^E_{exp(i)}$ are the calculated and experimental values of the excess molar volume respectively, and N is the number of data points for each data set. Values of rmsd listed in Table 3 indicate good agreement between the calculated and experimental values.

Apparent molar volume (V_Φ) [10, 11] of solution of hydroquinone in pure solvents and binary solvent mixture was calculated by using eq.6

$$V_\Phi = 1000(d^0\text{-}d)/dd^0m + M/d \quad \ldots (6)$$

Where d is density of ternary solution, d^0 is density of binary solvent, m is malality of solution (moles/1000gm of solvent) and M is molecular weight of solute.

EXPERIMENTAL SECTIONS

Material: Triple distilled water was used in all experiments. Other chemicals was supplied by

Chemical Name	Supplier Name	Percentage purity	Standard
Hydroquinone	Sigma-Aldrich co.	99%	Reagent Grade
Ethanol	Merck, Germany.	≥99.8%	G.R.
1-Propanol	Spectrochem, Mumbai, India.	≥99.8%	HPLC

Apparatus and Procedure: The apparatus and procedures used for density measurement have been described earlier in detail [12-15]. Briefly in this work; an excess amount of hydroquinone was added to

the binary solvents mixtures prepared by weight (Shimadzu, Auxzzo) with an uncertainty of ± 0.1 mg, in a specially designed 100 ml jacketed flask. Water was circulated at constant temperature between the outer and inner walls of the flask. The temperature of the circulating water was controlled by thermostat to within (± 0.1) K. The solution was continuously stirred using a magnetic stirrer for sufficient time (about 3hr) so that equilibrium is assured, no further solute dissolved, and the temperature of solution is same as that of circulating water; the stirrer was switched off and the solution was allowed to stand for 1hr. Then 5 ml of the supernatant liquid was withdrawn from the flask in a weighing bottle with the help of pipette which is hotter than the solution. Solutions were dried gravimetrically till constant weight of weighing bottle was reached. Molality(*m*) of hydroquinone was calculated by constant weights of solute. This flask solution was used to fill bicapillary pycnometer.

Densities were determined using a 15 cm^3 bicapillary pycnometer as described earlier [16-18]. For calibration of pycnometer triply distilled and degassed water with a density of 0.99705 $g \cdot cm^{-3}$ at 298.15 K was used. The filled pycnometer (without air bubble) with experimental liquids was kept in a transparent walled thermostat maintained at constant temperature (±0.1 K) for 10 to 15 min to attain thermal equilibrium. The heights of the liquid levels in the two arms were measured with the help of a travelling microscope, which could read to 0.01 mm. The estimated standard uncertainty of the density measurements of the solvent and binary mixtures was 10 $kg \cdot m^{-3}$.

RESULTS AND DISCUSSIONS

The experimental values of densities (ρ) of pure water, ethanol, 1-propanol and water+ethanol, water+1-propanol binary solvents also the densities of the saturated solutions of hydroquinone in water, ethanol, 1-propanol and their binary mixtures water+ethanol, water+1-propanol have been experimentally measured at temperatures (293.15, 295.65, 298.15, 300.65, 303.15, 305.65, 308.15, 310.65, 313.15) K. Excess molar volumes (V^E) data were correlated with values obtained from Redlich−Kister, apparent molar volume (V_Φ) are given in Table-1 & 2. Calculated partial excess molar volumes at infinite dilution ($\bar{V}_i^{E,\infty}$) at T = (293.15 to 313.15) K from Redlich−Kister Parameters *Ai* shown in Table 4. Negative contribution of V^E may arise from following effects

- Strong interactions between water and alcohol, which enhance the solvent structure in the mixtures.
- Breaking of inter-molecular hydrogen-bonded structure of water by the addition of alcohol to form new intermolecular hydrogen-bond which gives a more compact structure as well as geometrical effects such as interstitial accommodation, making V^E negative.
- As added ethanol fill up the all interstitial space between water molecules from 0.1 to 0.4 mole fraction ethanol further addition of ethanol from 0.4 to 0.6 there is change in volume V^E remains constant. After 0.6 mole fraction of ethanol, V^E values start to increase.(Fig.1)
- The highest negative V^E values for water+1-propanol are noticeably observed at only 0.5 mole fraction of 1-propanol.(Fig. 2)
- From above observations we say that ethanol is more associative with water than 1-propanol. As V^E values of water+ethanol are more negative than water+1-propanol.

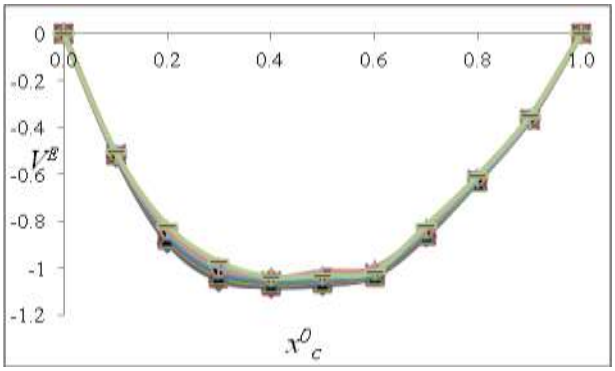


Fig.1: Excess molar volumes (V^E) vs. Mole fraction of Ethanol (x_c^0) at Temperatures (◆T=293.15 K, ■T=295.15 K; ▲T=298.15K; ×T=300.15 K; ○T=303.15 K; ●T=305.15 K; +T=308.15 K; -T=310.15 K & ▬ T=313.15 K).

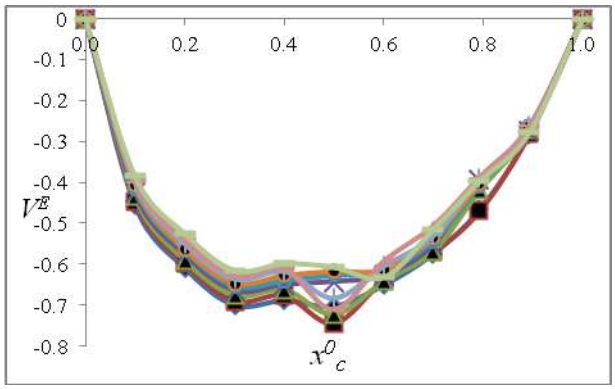


Fig.2: Excess molar volumes (V^E) vs. Mole fraction of 1-Propanol (x_c^0) at Temperatures (◆T=293.15 K, ■T=295.15 K; ▲T=298.15K; ×T=300.15 K; ○T=303.15 K; ●T=305.15 K; +T=308.15 K; -T=310.15 K & ▬ T=313.15 K).

The positive value of V_Φ indicates weak solute-solvent interactions only in terms of H-bonding and not any strong electrostatic force of attractions. V_Φ values of hydroquinone in water are more than in alcohol, indicates hydroquinone interaction is stronger in alcohol than water. Hence hydroquinone is more soluble in alcohol than in water which is confirmed from *m* values in Table-1, 2 and Fig.3, 4.

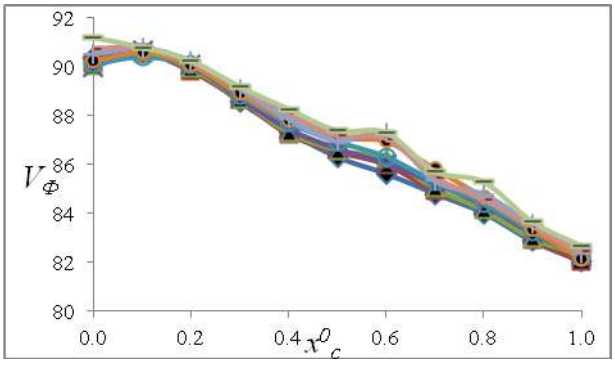


Fig.3: Apparent molar volume (V_Φ) of Hydroquinone vs. Mole fraction ethanol (x^0_C) at Temperatures (◆T=293.15 K, ■T=295.65 K; ▲T=298.15K; ×T=300.65 K; ○T=303.15 K; ●T=305.65 K; +T=308.15 K; -T=310.65 K & ▬T=313.15 K).

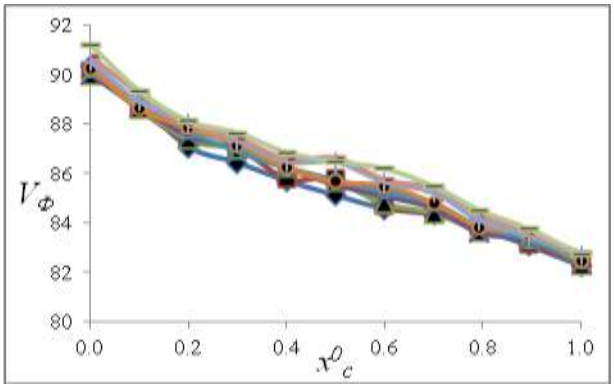


Fig.4: Apparent molar volume (V_Φ) of Hydroquinone vs. Mole fraction 1-propanol (x^0_C) at Temperatures (◆T=293.15 K, ■T=295.65 K; ▲T=298.15K; ×T=300.65 K; ○T=303.15 K; ●T=305.65 K; +T=308.15 K; - T=310.65 K & ▬T=313.15 K).

Molalities of hydroquinone are more in water+ethanol than in water+1-propanol. Higher *m* values observed at 0.6 mole fraction of ethanol and 0.4 mole fraction of 1-propanol then after *m* values were very slowly decreases. The decreasing trend of *m* of hydroquinone in pure solvent was ethanol > 1-propanol > water. Also *m* values continuously increased with increase in temperature at same mole fraction of alcohol (Fig.5, 6). For ternary system it was observed that V_Φ values slight more in ethanol system than in 1-propanol system, it is due to higher *m* values of hydroquinone in mole fractions of ethanol than mole fractions of 1-propanol.

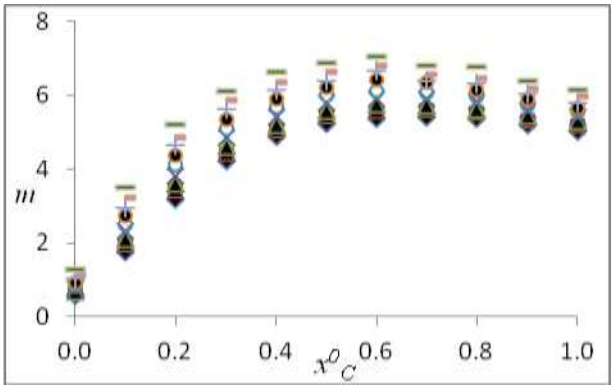


Fig.5: Plot of Molality(*m*) Vs. Mole Fraction of Ethanol(x_C) for Hydroquinone+ Water + Ethanol System.(◆T=293.15; ■ T =295.65; ▲ T =298.15; × T =300.65; ○ T =303.15; ● T =305.65;+ T =308.15; - T =310.65; ▬ T =313.15).

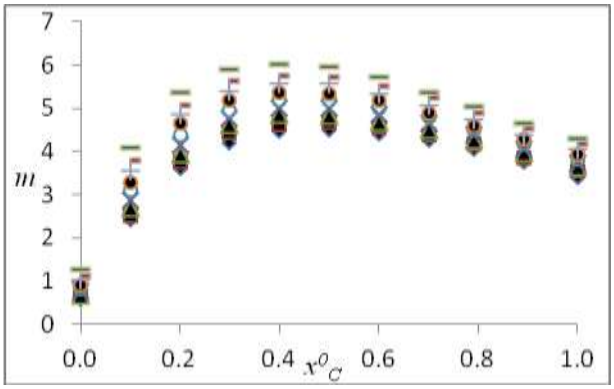
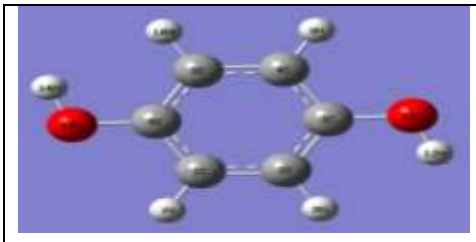


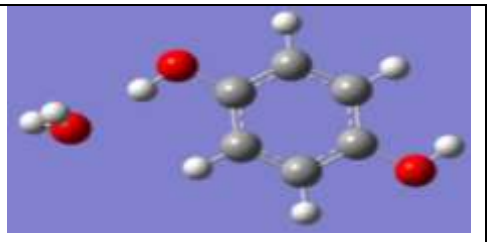
Fig.6: Plot of Molality(m) Vs. Mole Fraction of 1-Propanol(x^0_C) for Hydroquinone+ Water + 1-Propanol System.(◆T=293.15; ■ T =295.65; ▲ T =298.15; × T =300.65; ○ T =303.15; ● T =305.65;+ T =308.15; - T =310.65; ▬ T =313.15).

Computational study using Gaussian 09W software, DFT method, B3LYP 6-31(G)d as basis set was performed to understand the fundamental interactions between solvent-solvent and solute-solvent molecules. First, the structures of the solvent were optimized and stable conformers were obtained. The optimized structure of alcohols then interacted with water molecule and hydroquinone molecule as shown in Fig.7.

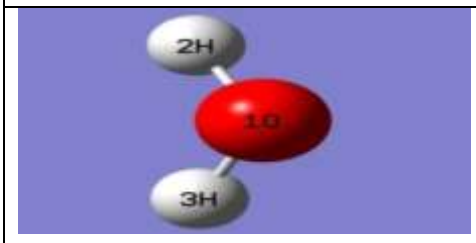
Fig.7: Optimized structures of solute, solvents combinations by DFT method at B3LYP level using 6-31G(d) basis set



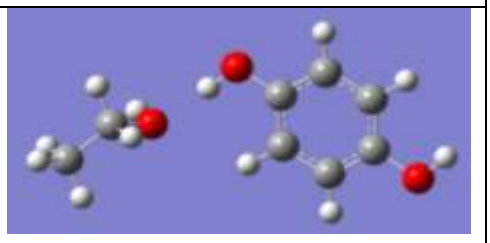
1-Optimized structure of **H**



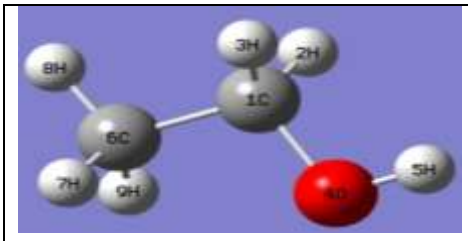
7-Optimized structure of **WH**



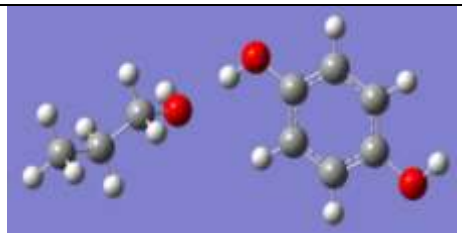
2-Optimized structure of **W**



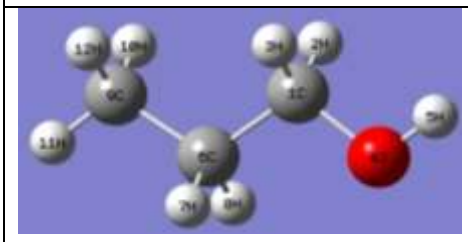
8-Optimized structure of **EH**



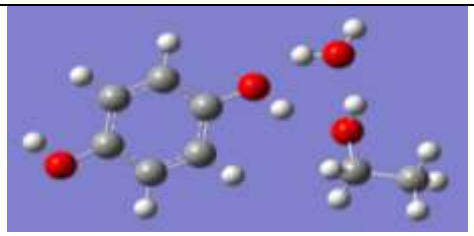
3-Optimized structure of **E**



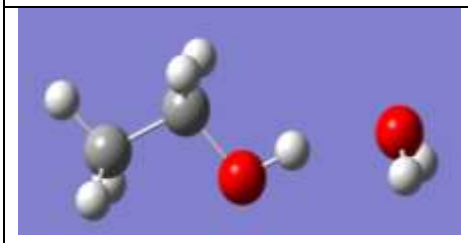
9-Optimized structure of **PH**



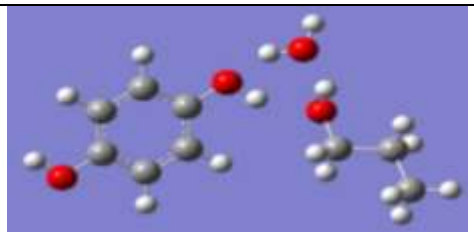
4-Optimized structure of **P**



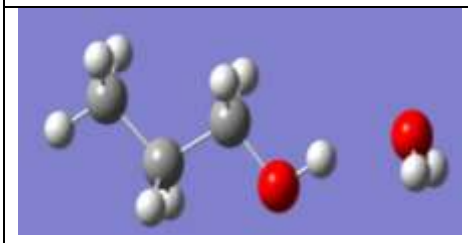
10- Optimized structure of **WEH**



5-Optimized structure of **WE**



11-Optimized structure of **WPH**



6-Optimized structure of **WP**

Dipole moment, total energy ,molecular symmetry , I.R. frequency of alcoholic –OH group, alcoholic –OH bond distance in angstroms unit and distance of intermolecular Hydrogen bonding present between alcohol with water and hydroquinone was given in Table 5.

Table 5-Calculated –OH str. freq. along with palarizability, dipole moment, -OH bond distance, intermolecular H-bond distance for pure substance, binary solvents & ternary solutions by DFT/B3LYP method at 6-31G (d) basis set

System	Phase/ Media	Dipole Moment (Debye)	(α) $Bohr^3$	Alcoholic υ-OH cm^{-1}	Alcoholic (-OH) Bond Dist. (^0A)	Intermolecular H-Bond Dist.(^0A)
H	Gas	0.001	64.14	3612.75(sym.str.) 3611.67uns.str.)	-	-
	Water	0.000	83.35	3598.54(sym.str.) 3597.4uns.str.)	-	-
W	Gas	2.0952	5.22	3584.18(sy.str.) 3701.29(Uns.str.)	-	-
	Water	2.3139	5.52	3584.78(sy.str.) 3684.62(Uns.str.)	-	-
E	Gas	1.5613	26.40	3607.31	0.96903	-
	Water	1.9063	31.37	3601.80	0.97008	-
P	Gas	1.488	36.84	3608.16	0.96895	-
	Water	1.8451	44.69	3602.54	0.96994	-
WE	Gas	2.2392	33.00	3469.99	0.97756	1.9054
	Water	3.4239	38.68	3381.81	0.98236	1.8355
WP	Gas	2.2959	43.49	3473.21	0.97722	1.9034
	Water	3.3881	52.02	3381.89	0.98230	1.8343
WH	Gas	3.5292	71.58	3408.1	-	1.8354
	Water	3.7993	91.46	3258.78	-	1.7647
EH	Gas	3.5584	93.71	3595.58	0.97060	1.8210
	Water	3.8025	118.08	3588.40	0.97175	1.7617
PH	Gas	3.6815	104.53	3595.81	0.97061	1.8231
	Water	3.8639	131.51	3591.26	0.97167	1.7637
WEH	Gas	1.3112	101.56	3318.50	0.98743	1.7901
	Water	1.6648	126.93	3290.69	0.98861	1.7796
WPH	Gas	1.3079	112.29	3319.03	0.98733	1.7901
	Water	1.7017	140.30	3291.71	0.98843	1.7814

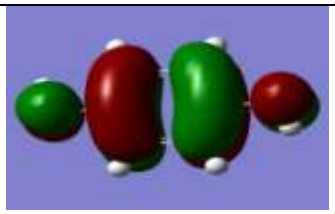
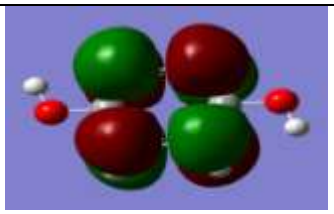
[Abbreviations:-W: Water, M: Methanol, E: Ethanol, P: 1-Propanol, H: Hydroquinone]

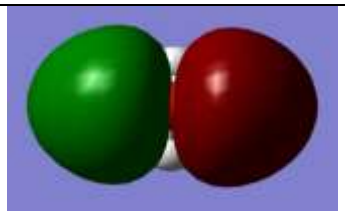
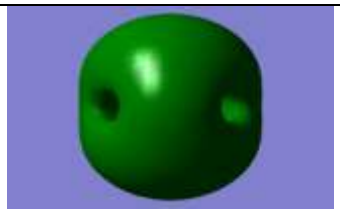
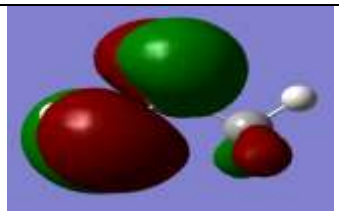
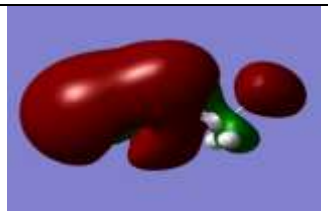
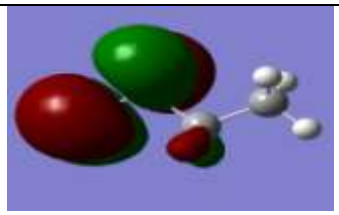
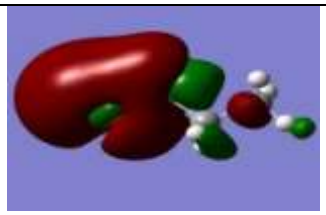
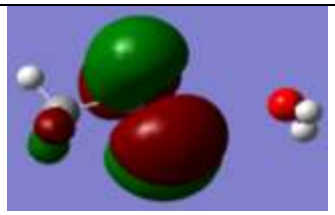
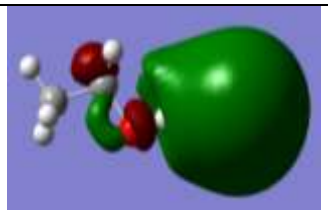
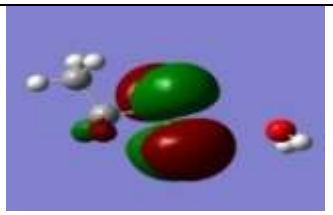
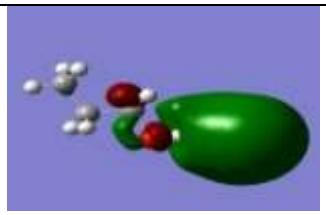
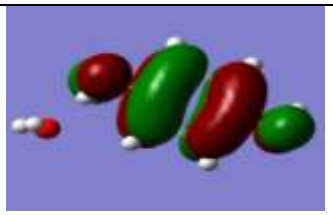
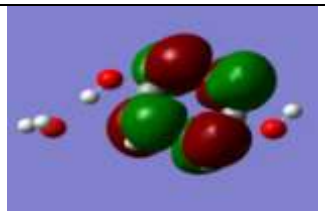
- HOMO-LUMO with energy gap between them is shown in Fig. 8. Energies of all optimized structure of HOMO, LUMO and their energy gap were shown in Table.6

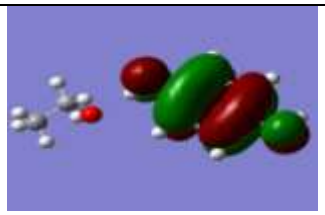
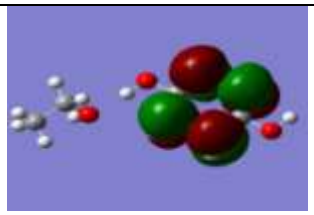
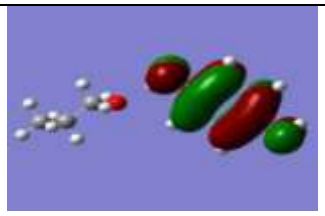
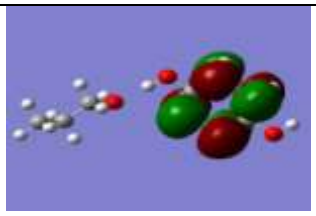
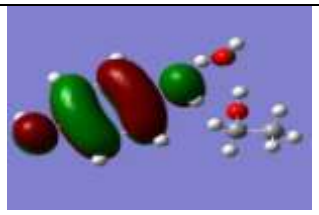
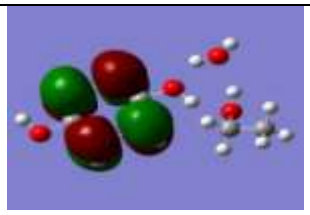
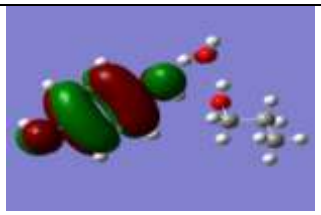
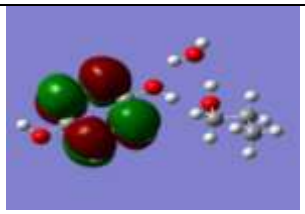
Table 6-HOMO, LUMO energies and Energy Gap between LUMO-HOMO Calculated by DFT method at B3LYP level using 6-31G (d) basis set.

System	Phase/Media	HOMO (eV)	LUMO (eV)	LUMO-HOMO Energy gap (eV)
H	Gas	-5.412	-0.062	5.350
	Water	-5.536	-0.174	5.361
W	Gas	-7.924	1.704	9.628
	Water	-8.035	2.062	10.097
E	Gas	-7.117	2.085	9.202
	Water	-7.205	2.301	9.505
P	Gas	-7.114	2.113	9.227
	Water	-7.210	2.328	9.538
WE	Gas	-6.501	1.039	7.540
	Water	-6.790	1.588	8.378
WP	Gas	-6.502	1.028	7.530
	Water	-6.794	1.588	8.382
WH	Gas	-4.926	0.365	5.290
	Water	-5.316	-0.036	5.280
EH	Gas	-4.900	0.381	5.281
	Water	-5.318	-0.036	5.282
PH	Gas	-4.890	0.391	5.281
	Water	-5.320	-0.037	5.283
WEH	Gas	-5.363	-0.004	5.359
	Water	-5.523	-0.162	5.361
WPH	Gas	-5.358	0.002	5.360
	Water	-5.526	-0.164	5.363

Fig. 8-HOMO, LUMO structures with LUMO-HOMO Energy Gap.

Molecule	HOMO	L-H E.G. (eV)	LUMO
H		Gas 5.350 Water 5.361	

W		Gas 9.628 Water 10.097	
E		Gas 9.202 Water 9.505	
P		Gas 9.227 Water 9.538	
WE		Gas 7.540 Water 8.378	
WP		Gas 7.530 Water 8.382	
WH		Gas 5.290 Water 5.280	

EH		Gas 5.281 Water 5.282	
PH		Gas 5.281 Water 5.283	
WEH		Gas 5.359 Water 5.361	
WPH		Gas 5.360	

The trend of energy gap is W> P≈E >WE≈WP >WPH≈WEH≈H >WH≈PH≈EH. From Table-6 we observed that solvent shows more energy gap than hydroquinone solutions those solvent-solvent system are more stable than solute-solute, solute-solvent system. Theoretical υ-OH cm^{-1} given in Table-5, its decreasing trend was H> P≈E >PH≈EH > W > WP >WE > WH > WPH≈WEH indicates that lower the υ-OH stronger the intermolecular H-bonding between them. This trend indicates that stronger interactions in ternary systems than binary systems.

CONCLUSIONS

The densities of pure, binary solvent systems were decreases with increase in mole fraction of alcohols and temperatures. In case of ternary solutions densities values were decreases with increase in mole fraction of alcohols and increases with temperatures this was due to increase of solubility in terms of molality. The molality (*m*) of hydroquinone in pure and binary solvent system was given in Table-1, 2. The trend of *m* in are shown as 0.6 WE > 0.4 WP > E > P >> W at same temperature, which explained

solubility rule 'like dissolved like'. Also these values of *m* increase with increase in temperature. As V^E are more negative at 0.4 to 0.6 mole fraction of ethanol, *m* values increase rapidly up to 0.6 mole fraction of ethanol then remains nearly same and very slowly decreases. The V^E are more negative at 0.5 mole fraction of 1-propanol, *m* values increase rapidly up to 0.4 & 0.5 mole fractions of 1-propanol then slowly decreases. From these result we say that solubility increase with mole fraction of alcohol but after 0.6 mole fraction of ethanol and 0.4 mole fraction of 1-propanol, addition of alcohol is less significant for solubility of hydroquinone.

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