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Molecular Interactions in Binary Solvent Mixtures and Catechol in Pure, Binary Solvent Mixtures at 293.15. to 313.15 K with DFT Study

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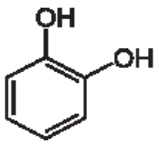
ABSTRACT

Density of water, methanol, ethanol,1-propanol and water+methanol, water+ethanol, water +1-propanol binary solvent in pure form were experimentally measured. In these same series of solvent catechol was added to make saturated solutions of catechol in water, methanol, ethanol, 1-propanol and their binary mixtures water+methanol, water+ethanol, water+1-propanol have been experimentally measured for comparative studies at (293.15 to 313.15) K temperatures and experimental density data used to calculate the excess molar volumes (V^E), apparant molar volume (V_Φ). 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 ($\bar{V}_i^{E,\infty}$). Solvent-solvent and solute-solvent interaction was explain by using Gaussian 09 software, method applied was DFT, B3LYP 6-31(G)d.

Keyword: DFT, Hydroquinone, Density, Excess molar volumes(V^E), Apparant molar volume (V_Φ).

I. INTRODUCTION

Theoretical calculation done by Gaussian 09 software is now very good applicable in chemistry for interpretation of structure of various organic molecules [1,2]. Here we used same for explaining interaction with molecule. Phenolic compounds were reported as antibacterial activity in various plants. Catechol and pyrogallol are allelochemicals which belong to phenolic compounds synthesized in plants. Their antimicrobial activities were investigated on three bacteria (Pseudomonas putida, Pseudomonas pyocyanea, Corynebacterium xerosis) and two fungi (Fusarium oxysporum, Penicillium italicum) phytopathogenic species [3]. Catechol is used in organic synthesis as precursor, polymer and dyes industries [4]. The molecular structure of a catechol is as follows



Catechol is white to brown crystallaline solid flakes. IUPAC name of Catechol is benzene 1,2-diol, with the molecular formula $C_6H_6O_2$.. Molar mass is 110.11gm/mol, melting point is about 105^0C. Solvent-solvent and solvent-solute interactions of electrolytes are extremely important for the synthesis, design of processes and simulations of unit operations [5].Density of catechol in pure water, alcohols at certain temperatures were available but in water–alcohol mixed solvent system for 0.1 to 0.9 mole fraction of methanol, ethanol and 1-propanol have to be investigate. We have undertaken the measurements of densities of pure solvents, binary solvent mixtures and saturated solutions of catechol in water + methanol, water + ethanol,water+1-propanol binary solvents over the entire composition range from 0 to 1 mole fraction of methanol, ethanol. The experimental work was carried out at (293.15 to 313.15) K and Excess molar volumes (V^E)[6] were calculated from the measured densities of the pure components and the binary mixtures as shown in Table 1,2,3 using eq.1.

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

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 + methanol binary system and molality (m), density (ρ), apparant molar volume (V_Φ) of catechol + water + methanol 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	4.5152	1.0732	87.0814
0.1000	0.9714	-0.3021	-0.3027	8.5665	1.0986	86.3277
0.2000	0.9497	-0.6094	-0.6058	11.3172	1.1021	87.0467
0.3011	0.9280	-0.8371	-0.8434	12.5985	1.0989	86.8971
0.4000	0.9075	-0.9857	-0.9771	13.3604	1.0957	86.3296
0.5054	0.8842	-0.9926	-1.0067	13.4093	1.0907	84.9937
0.5999	0.8652	-0.9549	-0.9455	14.1068	1.0854	84.8244
0.7012	0.8448	-0.8096	-0.8065	13.7044	1.0795	83.2306
0.8021	0.8259	-0.6021	-0.6067	13.9788	1.0746	82.4106
0.9002	0.8088	-0.3524	-0.3515	14.4969	1.0691	82.2317
1.0000	0.7916	0.0000	0.0000	16.6892	1.0647	84.0035
			295.65 K			
0.0000	0.9977	0.0000	0.0000	5.4104	1.0828	87.1352
0.1000	0.9706	-0.3051	-0.3058	9.0000	1.1027	86.1485
0.2000	0.9483	-0.6099	-0.6064	12.3817	1.1042	87.6990
0.3011	0.9264	-0.8381	-0.8411	13.0915	1.1013	86.8865
0.4000	0.9053	-0.9751	-0.9740	13.7408	1.0969	86.3400
0.5054	0.8824	-0.9973	-1.0051	14.0069	1.0923	85.2609
0.5999	0.8631	-0.9536	-0.9460	14.4535	1.0869	84.7970
0.7012	0.8427	-0.8116	-0.8082	14.1275	1.0812	83.3155
0.8021	0.8237	-0.6021	-0.6071	14.2421	1.0753	82.4462
0.9002	0.8065	-0.3507	-0.3497	15.0404	1.0697	82.6559
1.0000	0.7893	0.0000	0.0000	16.9629	1.0653	84.0111
			298.15 K			
0.0000	0.9970	0.0000	0.0000	6.4142	1.0911	87.4415
0.1000	0.9698	-0.3109	-0.3119	9.5399	1.1072	86.0402
0.2000	0.9471	-0.6142	-0.6086	13.7247	1.1081	88.1831
0.3011	0.9246	-0.8343	-0.8402	13.7189	1.1049	86.7923
0.4000	0.9034	-0.9763	-0.9737	14.5907	1.0999	86.5579

0.5054	0.8803	-0.9964	-1.0074	14.4928	1.0937	85.3880
0.5999	0.8611	-0.9620	-0.9504	15.1403	1.0885	85.1385
0.7012	0.8406	-0.8164	-0.8132	14.8026	1.0826	83.7463
0.8021	0.8214	-0.6050	-0.6113	14.4925	1.0767	82.3573
0.9002	0.8042	-0.3539	-0.3526	15.3352	1.0713	82.5631
1.0000	0.7870	0.0000	0.0000	17.8011	1.0662	84.5854
			300.65 K			
0.0000	0.9964	0.0000	0.0000	8.0228	1.0997	88.3729
0.1000	0.9688	-0.3139	-0.3150	10.0523	1.1137	85.5115
0.2000	0.9456	-0.6159	-0.6104	14.3591	1.1112	88.1132
0.3011	0.9228	-0.8373	-0.8418	14.2790	1.1062	86.9606
0.4000	0.9013	-0.9759	-0.9767	15.1435	1.1016	86.6386
0.5054	0.8783	-1.0045	-1.0124	14.9244	1.0963	85.2678
0.5999	0.8588	-0.9667	-0.9562	15.8635	1.0907	85.3540
0.7012	0.8382	-0.8217	-0.8184	15.3552	1.0842	83.9385
0.8021	0.8190	-0.6085	-0.6149	15.3645	1.0789	82.9090
0.9002	0.8017	-0.3557	-0.3544	16.2889	1.0731	83.2341
1.0000	0.7844	0.0000	0.0000	18.7531	1.0678	85.0804
			303.15 K			
0.0000	0.9957	0.0000	0.0000	9.3764	1.1089	88.3522
0.1000	0.9678	-0.3184	-0.3192	10.8581	1.1167	85.9102
0.2000	0.9441	-0.6187	-0.6147	15.1566	1.1146	88.1038
0.3011	0.9211	-0.8424	-0.8456	15.1139	1.1089	87.1341
0.4000	0.8994	-0.9810	-0.9804	15.7319	1.1041	86.6293
0.5054	0.8761	-1.0073	-1.0165	16.2342	1.0977	86.1114
0.5999	0.8566	-0.9720	-0.9612	17.7001	1.0916	86.6733
0.7012	0.8359	-0.8270	-0.8252	15.6503	1.0854	83.8747
0.8021	0.8167	-0.6190	-0.6240	15.7708	1.0803	82.9737
0.9002	0.7993	-0.3647	-0.3637	17.7646	1.0743	84.4659
1.0000	0.7818	0.0000	0.0000	20.0222	1.0696	85.7605
			305.65 K			
0.0000	0.9949	0.0000	0.0000	10.7384	1.1158	88.5425
0.1000	0.9665	-0.3164	-0.3169	12.2878	1.1206	86.6865
0.2000	0.9427	-0.6204	-0.6172	15.6812	1.1166	88.0673
0.3011	0.9194	-0.8439	-0.8486	15.8078	1.1112	87.2111
0.4000	0.8975	-0.9850	-0.9816	16.9396	1.1057	87.2052
0.5054	0.8740	-1.0113	-1.0185	17.0031	1.0995	86.3456
0.5999	0.8545	-0.9778	-0.9679	18.7135	1.0946	86.8814
0.7012	0.8338	-0.8335	-0.8376	16.1960	1.0875	83.9781
0.8021	0.8147	-0.6362	-0.6364	16.7227	1.0811	83.7678
0.9002	0.7970	-0.3683	-0.3681	18.6081	1.0762	84.8186
1.0000	0.7794	0.0000	0.0000	20.4879	1.0709	85.7672

308.15 K						
0.0000	0.9940	0.0000	0.0000	12.0244	1.1224	88.5398
0.1000	0.9656	-0.3254	-0.3256	13.4446	1.1231	87.2391
0.2000	0.9413	-0.6252	-0.6239	16.6414	1.1196	88.1774
0.3011	0.9177	-0.8478	-0.8506	16.7486	1.1137	87.4238
0.4000	0.8957	-0.9883	-0.9800	19.0315	1.1080	88.1330
0.5054	0.8715	-0.9974	-1.0157	17.6878	1.1011	86.4705
0.5999	0.8525	-0.9819	-0.9657	19.5754	1.0952	87.2574
0.7012	0.8315	-0.8332	-0.8365	18.0045	1.0886	85.3694
0.8021	0.8124	-0.6344	-0.6360	18.4374	1.0821	85.1101
0.9002	0.7947	-0.3682	-0.3677	19.9928	1.0777	85.6508
1.0000	0.7771	0.0000	0.0000	21.6581	1.0730	86.2412
310.65 K						
0.0000	0.9932	0.0000	0.0000	13.9047	1.1280	88.9617
0.1000	0.9644	-0.3278	-0.3275	15.0964	1.1275	87.7267
0.2000	0.9397	-0.6270	-0.6276	17.1766	1.1224	88.0175
0.3011	0.9158	-0.8488	-0.8526	17.0944	1.1158	87.2352
0.4000	0.8936	-0.9899	-0.9782	19.9188	1.1093	88.3432
0.5054	0.8694	-1.0011	-1.0110	19.1871	1.1026	87.1813
0.5999	0.8496	-0.9613	-0.9618	21.8414	1.0973	88.1789
0.7012	0.8294	-0.8418	-0.8375	18.5296	1.0903	85.4128
0.8021	0.8101	-0.6418	-0.6433	20.1225	1.0853	85.9055
0.9002	0.7925	-0.3773	-0.3772	20.7668	1.0798	85.8050
1.0000	0.7747	0.0000	0.0000	22.2909	1.0752	86.2226
313.15 K						
0.0000	0.9922	0.0000	0.0000	16.3974	1.1328	89.5678
0.1000	0.9632	-0.3308	-0.3316	16.5458	1.1303	88.1408
0.2000	0.9381	-0.6292	-0.6259	17.9036	1.1254	87.9332
0.3011	0.9140	-0.8511	-0.8536	17.7686	1.1184	87.1909
0.4000	0.8916	-0.9931	-0.9871	21.3279	1.1122	88.5718
0.5054	0.8671	-0.9997	-1.0247	21.2172	1.1060	87.8173
0.5999	0.8482	-0.9973	-0.9726	22.3845	1.0988	88.1956
0.7012	0.8269	-0.8405	-0.8415	20.0166	1.0930	86.0369
0.8021	0.8076	-0.6386	-0.6447	21.2029	1.0871	86.2689
0.9002	0.7901	-0.3845	-0.3832	22.6330	1.0811	86.8036
1.0000	0.7722	0.0000	0.0000	22.8261	1.0764	86.2613

[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}.

Table 2- Mole fraction of ethanol (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), apparant molar

volume (V_Φ) of catechol + 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	4.5152	1.0732	87.0814
0.0719	0.9726	-0.3429	-0.3481	8.9430	1.0955	87.6031
0.1483	0.9522	-0.7245	-0.7019	10.6966	1.0946	87.8277
0.2300	0.9287	-0.9542	-0.9617	12.1342	1.0904	87.8158
0.3168	0.9049	-1.0617	-1.0854	12.7007	1.0826	87.4269
0.4104	0.8821	-1.0845	-1.0896	12.7443	1.0739	86.6529
0.5089	0.8615	-1.0370	-1.0245	12.5906	1.0662	85.5683
0.6187	0.8426	-0.9568	-0.9295	12.8845	1.0553	85.7628
0.7358	0.8245	-0.7668	-0.7920	12.9550	1.0446	85.6862
0.8622	0.8081	-0.5109	-0.5067	12.4324	1.0349	82.3647
1.0000	0.7905	0.0000	0.0000	12.0289	1.0224	83.8404
			295.65 K			
0.0000	0.9977	0.0000	0.0000	5.4104	1.0828	87.1352
0.0719	0.9716	-0.3439	-0.3491	9.7921	1.0997	87.8867
0.1483	0.9506	-0.7191	-0.6970	11.3875	1.0984	87.8139
0.2300	0.9268	-0.9462	-0.9526	12.6294	1.0928	87.7776
0.3168	0.9028	-1.0529	-1.0770	13.4883	1.0846	87.7482
0.4104	0.8800	-1.0784	-1.0854	13.4943	1.0758	87.0327
0.5089	0.8595	-1.0398	-1.0242	13.2519	1.0667	86.1669
0.6187	0.8404	-0.9560	-0.9307	13.8670	1.0567	86.6274
0.7358	0.8224	-0.7700	-0.7945	13.4513	1.0461	85.9198
0.8622	0.8060	-0.5193	-0.5152	12.6295	1.0351	82.4075
1.0000	0.7882	0.0000	0.0000	12.2351	1.0236	83.7251
			298.15 K			
0.0000	0.9970	0.0000	0.0000	6.4142	1.0911	87.4415
0.0719	0.9706	-0.3438	-0.3488	10.6787	1.1043	88.0323
0.1483	0.9490	-0.7117	-0.6910	12.3688	1.1012	88.2182
0.2300	0.9249	-0.9379	-0.9413	13.2423	1.0954	87.8147
0.3168	0.9005	-1.0366	-1.0637	14.3270	1.0871	87.9880
0.4104	0.8779	-1.0697	-1.0735	14.1015	1.0781	87.1392
0.5089	0.8572	-1.0267	-1.0150	14.1186	1.0687	86.6877
0.6187	0.8383	-0.9517	-0.9236	14.7875	1.0583	87.2747
0.7358	0.8202	-0.7632	-0.7887	14.1701	1.0474	86.4685
0.8622	0.8038	-0.5166	-0.5124	13.1064	1.0373	82.6443

1.0000	0.7861	0.0000	0.0000	12.8169	1.0256	84.1784
			300.65 K			
0.0000	0.9964	0.0000	0.0000	8.0228	1.0997	88.3729
0.0719	0.9696	-0.3454	-0.3496	11.9162	1.1091	88.3901
0.1483	0.9471	-0.7025	-0.6849	13.3335	1.1048	88.3667
0.2300	0.9228	-0.9261	-0.9295	14.2439	1.0977	88.1820
0.3168	0.8983	-1.0278	-1.0503	15.3050	1.0892	88.3431
0.4104	0.8755	-1.0570	-1.0612	15.2125	1.0798	87.7709
0.5089	0.8548	-1.0173	-1.0030	14.9838	1.0703	87.1543
0.6187	0.8355	-0.9276	-0.9094	15.2980	1.0602	87.2853
0.7358	0.8177	-0.7554	-0.7744	14.9387	1.0494	86.8560
0.8622	0.8014	-0.5114	-0.5082	13.8439	1.0391	83.3159
1.0000	0.7837	0.0000	0.0000	13.3434	1.0273	84.5188
			303.15 K			
0.0000	0.9957	0.0000	0.0000	9.3764	1.1089	88.3522
0.0719	0.9684	-0.3454	-0.3495	12.9665	1.1130	88.5898
0.1483	0.9453	-0.6965	-0.6792	14.8123	1.1084	88.8313
0.2300	0.9206	-0.9154	-0.9189	15.8017	1.1000	88.8942
0.3168	0.8961	-1.0192	-1.0390	16.5730	1.0912	88.8752
0.4104	0.8732	-1.0473	-1.0535	15.9056	1.0818	87.8906
0.5089	0.8524	-1.0088	-1.0007	15.7619	1.0720	87.4663
0.6187	0.8335	-0.9383	-0.9108	15.5789	1.0620	87.1154
0.7358	0.8153	-0.7518	-0.7752	15.6651	1.0514	87.1506
0.8622	0.7990	-0.5098	-0.5061	14.5097	1.0405	83.8563
1.0000	0.7813	0.0000	0.0000	13.9772	1.0291	84.9539
			305.65 K			
0.0000	0.9949	0.0000	0.0000	10.7384	1.1158	88.5425
0.0719	0.9673	-0.3456	-0.3495	14.2206	1.1166	88.8847
0.1483	0.9437	-0.696	-0.6735	15.9487	1.1104	89.1885
0.2300	0.9186	-0.9052	-0.9081	16.9891	1.1019	89.2654
0.3168	0.8940	-1.0069	-1.0267	17.4032	1.0935	88.9677
0.4104	0.8710	-1.0385	-1.0426	17.2716	1.0841	88.5009
0.5089	0.8502	-0.9991	-0.9917	16.7104	1.0735	87.9399
0.6187	0.8312	-0.9273	-0.9024	16.2892	1.0633	87.4320
0.7358	0.8132	-0.7463	-0.7676	16.3065	1.0529	87.4039
0.8622	0.7969	-0.5072	-0.5038	14.9789	1.0419	84.0854
1.0000	0.7792	0.0000	0.0000	14.7073	1.0317	85.3672
			308.15 K			
0.0000	0.9940	0.0000	0.0000	12.0244	1.1224	88.5398
0.0719	0.9661	-0.3480	-0.3518	15.4739	1.1207	89.0285
0.1483	0.9420	-0.6865	-0.6708	17.1401	1.1132	89.3949
0.2300	0.9167	-0.9001	-0.9020	18.0011	1.1046	89.3824

0.3168	0.8920	-1.0026	-1.0212	18.6217	1.0952	89.3725
0.4104	0.8689	-1.0317	-1.0395	18.0595	1.0867	88.5555
0.5089	0.8482	-0.9978	-0.9890	17.8284	1.0754	88.4134
0.6187	0.8290	-0.9237	-0.8970	17.0410	1.0654	87.6526
0.7358	0.8109	-0.7401	-0.7628	17.1879	1.0548	87.8048
0.8622	0.7948	-0.5139	-0.5103	16.0084	1.0449	84.7748
1.0000	0.7771	0.0000	0.0000	15.3133	1.0340	85.6026
			310.65 K			
0.0000	0.9932	0.0000	0.0000	13.9047	1.1280	88.9617
0.0719	0.9649	-0.3484	-0.3520	17.3779	1.1243	89.4841
0.1483	0.9403	-0.6810	-0.6662	18.4127	1.1160	89.5745
0.2300	0.9147	-0.8920	-0.8931	19.2055	1.1069	89.5973
0.3168	0.8898	-0.9930	-1.0117	19.9800	1.0976	89.6674
0.4104	0.8667	-1.0221	-1.0333	19.1054	1.0881	88.9031
0.5089	0.8463	-1.0059	-0.9873	18.9657	1.0778	88.7867
0.6187	0.8268	-0.9139	-0.8977	18.2991	1.0670	88.3092
0.7358	0.8088	-0.7422	-0.7603	17.9529	1.0568	88.0279
0.8622	0.7925	-0.5054	-0.5023	16.5619	1.0474	84.8490
1.0000	0.7749	0.0000	0.0000	15.9224	1.0364	85.7944
			313.15 K			
0.0000	0.9922	0.0000	0.0000	16.3974	1.1328	89.5678
0.0719	0.9635	-0.3461	-0.3503	18.9891	1.1270	89.7702
0.1483	0.9383	-0.6728	-0.6565	20.2099	1.1187	89.9291
0.2300	0.9125	-0.8800	-0.8788	20.8425	1.1089	89.9886
0.3168	0.8874	-0.9773	-0.9985	20.8118	1.0998	89.6608
0.4104	0.8643	-1.0077	-1.0234	20.6446	1.0899	89.4194
0.5089	0.8439	-0.9944	-0.9780	20.0217	1.0803	88.9815
0.6187	0.8246	-0.9141	-0.8849	19.4950	1.0692	88.7567
0.7358	0.8063	-0.7220	-0.7483	19.0271	1.0595	88.3527
0.8622	0.7904	-0.5101	-0.5058	17.2616	1.0483	85.3295
1.0000	0.7727	0.0000	0.0000	16.9868	1.0396	86.3592

[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}.

Table 3- 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), apparant molar volume (V_Φ) of catechol + 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$^-$	$V^E_{(Exp.)}$ 10^6.m^3.mol$^-$	$V^E_{(Cal.)}$ 10^6.m^3.mol$^-$	m mol.Kg^{-1}	Ternary solution $\rho.10^{-3}$/ kg.m^{-3}	V_Φ m^3.mol^{-1}

	3	1	1			
			293.15 K			
0.0000	0.9982	0.0000	0.0000	4.5152	1.0733	87.0769
0.1000	0.9551	-0.4566	-0.4570	10.5340	1.0942	87.9938
0.2001	0.9180	-0.6102	-0.6092	12.0619	1.0826	87.9726
0.2999	0.8913	-0.7005	-0.6875	12.5313	1.0698	87.9896
0.4001	0.8697	-0.6902	-0.7427	12.2935	1.0562	87.7305
0.5226	0.8535	-0.8423	-0.7479	12.0540	1.0445	87.6506
0.6000	0.8407	-0.6495	-0.7010	10.7231	1.0326	86.0100
0.6998	0.8297	-0.5730	-0.5930	10.9619	1.0209	87.2654
0.8002	0.8205	-0.4777	-0.4589	10.3261	1.0101	86.8436
0.8999	0.8118	-0.2983	-0.3011	9.6285	0.9999	86.0450
1.0000	0.8032	0.0000	0.0000	8.4000	0.9890	83.5006
			295.65 K			
0.0000	0.9977	0.0000	0.0000	5.4104	1.0828	87.1352
0.1000	0.9535	-0.4459	-0.4467	11.2229	1.0970	88.1560
0.2001	0.9161	-0.5984	-0.5958	12.5989	1.0845	88.0738
0.2999	0.8892	-0.6897	-0.6766	12.9792	1.0712	88.0731
0.4001	0.8676	-0.6783	-0.7344	12.9026	1.0580	87.9895
0.5226	0.8513	-0.8330	-0.7382	12.4288	1.0454	87.7879
0.6000	0.8385	-0.6386	-0.6894	11.3692	1.0342	86.6198
0.6998	0.8276	-0.5671	-0.5830	11.2854	1.0227	87.2351
0.8002	0.8183	-0.4740	-0.4590	10.7812	1.0116	87.1843
0.8999	0.8098	-0.3118	-0.3140	10.1655	1.0015	86.6892
1.0000	0.8011	0.0000	0.0000	9.2240	0.9908	85.2191
			298.15 K			
0.0000	0.9970	0.0000	0.0000	6.4142	1.0911	87.4415
0.1000	0.9519	-0.4358	-0.4374	12.1429	1.0999	88.4670
0.2001	0.9144	-0.5904	-0.5838	13.3510	1.0870	88.2874
0.2999	0.8872	-0.6765	-0.6654	13.8923	1.0734	88.5059
0.4001	0.8656	-0.6657	-0.7254	13.3857	1.0600	88.0438
0.5226	0.8493	-0.8246	-0.7324	12.5780	1.0478	87.3448
0.6000	0.8366	-0.6397	-0.6849	12.0110	1.0359	87.1541
0.6998	0.8256	-0.5665	-0.5785	11.6582	1.0239	87.4210
0.8002	0.8162	-0.4627	-0.4530	11.1627	1.0130	87.3624
0.8999	0.8078	-0.3061	-0.3073	10.5721	1.0027	87.0398
1.0000	0.7991	0.0000	0.0000	9.6291	0.9919	85.7348
			300.65 K			
0.0000	0.9964	0.0000	0.0000	8.0228	1.9997	88.3729
0.1000	0.9502	-0.4266	-0.4281	13.1781	1.1039	88.6293
0.2001	0.9123	-0.5771	-0.5706	14.2348	1.0899	88.4852
0.2999	0.8851	-0.6647	-0.6529	14.4886	1.0762	88.4585

0.4001	0.8633	-0.6524	-0.7149	14.1356	1.0615	88.4267
0.5226	0.8471	-0.8199	-0.7222	13.0697	1.0493	87.5391
0.6000	0.8343	-0.6261	-0.6734	12.3322	1.0372	87.1490
0.6998	0.8232	-0.5502	-0.5653	12.1876	1.0261	87.5931
0.8002	0.8138	-0.4530	-0.4410	11.4718	1.0152	87.2077
0.8999	0.8054	-0.2994	-0.3009	10.9814	1.0049	87.1256
1.0000	0.7968	0.0000	0.0000	9.9668	0.9939	85.8152
			303.15 K			
0.0000	0.9957	0.0000	0.0000	9.3764	1.1089	88.3522
0.1000	0.9484	-0.4154	-0.4169	14.1325	1.1068	88.8142
0.2001	0.9103	-0.5667	-0.5603	15.1493	1.0923	88.7260
0.2999	0.8830	-0.6540	-0.6428	15.3791	1.0789	88.6819
0.4001	0.8611	-0.6416	-0.7029	14.7276	1.0642	88.4147
0.5226	0.8447	-0.8047	-0.7088	14.3081	1.0512	88.5047
0.6000	0.8320	-0.6163	-0.6616	12.9051	1.0389	87.4314
0.6998	0.8209	-0.5412	-0.5580	12.7815	1.0289	87.7532
0.8002	0.8116	-0.4512	-0.4384	11.9946	1.0174	87.4464
0.8999	0.8032	-0.2987	-0.3003	11.3315	1.0071	87.0812
1.0000	0.7946	0.0000	0.0000	10.2974	0.9959	85.8535
			305.65 K			
0.0000	0.9949	0.0000	0.0000	10.7384	1.1158	88.5425
0.1000	0.9468	-0.4075	-0.4098	15.2633	1.1099	89.0419
0.2001	0.9086	-0.5627	-0.5519	16.0070	1.0942	88.9660
0.2999	0.8810	-0.6457	-0.6363	16.0872	1.0804	88.8974
0.4001	0.8590	-0.6292	-0.6977	15.5386	1.0668	88.6190
0.5226	0.8428	-0.8032	-0.7021	14.5318	1.0544	88.0373
0.6000	0.8299	-0.6105	-0.6529	13.4623	1.0417	87.5052
0.6998	0.8187	-0.5314	-0.5490	13.1307	1.0299	87.8409
0.8002	0.8095	-0.4446	-0.4339	12.4430	1.0218	87.1250
0.8999	0.8012	-0.3021	-0.3032	11.6776	1.0087	87.1731
1.0000	0.7925	0.0000	0.0000	10.6360	0.9979	85.9256
			308.15 K			
0.0000	0.9940	0.0000	0.0000	12.0244	1.1224	88.5398
0.1000	0.9452	-0.4013	-0.4036	16.3432	1.1126	89.2262
0.2001	0.9066	-0.5496	-0.5398	16.8510	1.0969	89.0325
0.2999	0.8790	-0.6346	-0.6231	16.7793	1.0826	88.9635
0.4001	0.8570	-0.6182	-0.6868	15.9299	1.0681	88.6157
0.5226	0.8407	-0.7913	-0.6936	14.9841	1.0560	88.0801
0.6000	0.8279	-0.6019	-0.6445	14.0157	1.0419	87.9871
0.6998	0.8168	-0.5271	-0.5395	13.8025	1.0320	88.1995
0.8002	0.8074	-0.4320	-0.4245	12.9684	1.0227	87.5520
0.8999	0.7992	-0.2969	-0.2975	12.1958	1.0111	87.4054

1.0000	0.7905	0.0000	0.0000	10.9998	0.9994	86.1344
			310.65 K			
0.0000	0.9932	0.0000	0.0000	13.9047	1.1280	88.9617
0.1000	0.9436	-0.3959	-0.3980	17.7032	1.1153	89.5101
0.2001	0.9047	-0.5416	-0.5323	18.2272	1.1000	89.3393
0.2999	0.8770	-0.6282	-0.6170	17.6875	1.0847	89.1695
0.4001	0.8549	-0.6117	-0.6811	17.1422	1.0706	89.0977
0.5226	0.8386	-0.7869	-0.6841	16.0591	1.0575	88.7581
0.6000	0.8257	-0.5898	-0.6314	14.9087	1.0457	88.2117
0.6998	0.8144	-0.5024	-0.5251	14.5453	1.0344	88.4879
0.8002	0.8053	-0.4306	-0.4165	13.6478	1.0239	88.1195
0.8999	0.7971	-0.2992	-0.3008	12.9386	1.0133	87.9853
1.0000	0.7884	0.0000	0.0000	11.7115	1.0032	86.5848
			313.15 K			
0.0000	0.9922	0.0000	0.0000	16.3974	1.1328	89.5678
0.1000	0.9417	-0.3859	-0.3890	18.7309	1.1184	89.4973
0.2001	0.9025	-0.5260	-0.5126	19.6075	1.1024	89.6290
0.2999	0.8748	-0.6148	-0.6018	18.7665	1.0873	89.3666
0.4001	0.8526	-0.6006	-0.6802	18.0800	1.0728	89.3233
0.5226	0.8366	-0.7920	-0.6982	16.3404	1.0603	88.4052
0.6000	0.8241	-0.6305	-0.6489	15.4600	1.0480	88.2966
0.6998	0.8123	-0.5120	-0.5412	15.2473	1.0365	88.7682
0.8002	0.8032	-0.4419	-0.4312	14.3514	1.0264	88.4218
0.8999	0.7951	-0.3156	-0.3162	13.1959	1.0157	87.7075
1.0000	0.7862	0.0000	0.0000	12.2617	1.0050	86.9831

[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}.

Table 4- Regressed Parameters Ai and correlation coefficient R^2 of the Redlich−Kister Equation and the Root-Mean-Square Deviation (σ)

TK	A_0 10^6.m^3·mol^{-1}	A_1 10^6.m^3·mol^{-1}	A_2 10^6.m^3·mol^{-1}	A_3 10^6.m^3·mol^{-1}	A_4 10^6.m^3·mol^{-1}	R^2	σ
			Methanol + Water				
293.15	-4.0313	0.375579	0.651781	-1.124917	-0.05850	0.977	0.007
295.65	-4.0245	0.332711	0.614002	-1.004775	-0.03276	0.987	0.004
298.15	-4.0331	0.279071	0.627285	-0.885691	-0.15558	0.967	0.007
300.65	-4.0527	0.246611	0.658473	-0.820775	-0.22206	0.972	0.006
303.15	-4.0691	0.235461	0.615839	-0.858874	-0.29901	0.976	0.005
305.65	-4.0763	0.177013	0.373861	-0.840942	0.06779	0.985	0.005
308.15	-4.0653	0.180141	0.293827	-0.747052	0.05244	0.937	0.009
310.65	-4.0468	0.206370	0.123298	-0.870343	0.11927	0.975	0.005

313.15	-4.1012	0.185917	0.477951	-0.858735	-0.43770	0.896	0.012
Ethanol + Water							
293.15	-4.1263	1.583482	-3.236329	-1.335992	3.34446	0.974	0.017
295.65	-4.1243	1.524171	-3.085615	-1.362513	2.98218	0.973	0.017
298.15	-4.0865	1.470175	-3.005502	-1.285261	2.81432	0.972	0.018
300.65	-4.0388	1.486559	-2.819718	-1.326054	2.42840	0.982	0.014
303.15	-4.0276	1.382664	-2.716541	-1.158751	2.29876	0.979	0.015
305.65	-3.9911	1.353850	-2.603786	-1.133264	2.06171	0.981	0.014
308.15	-3.9807	1.375678	-2.420626	-1.267727	1.60486	0.981	0.015
310.65	-3.9728	1.290451	-2.297105	-1.060603	1.52248	0.984	0.014
313.15	-3.9359	1.319145	-2.035061	-1.250187	0.96881	0.974	0.018
1-Propanol + Water							
293.15	-3.0162	0.391697	0.354396	1.081644	-3.47103	0.939	0.041
295.65	-2.9796	0.437733	0.490634	0.757984	-3.80860	0.935	0.041
298.15	-2.9544	0.389999	0.559019	0.805227	-3.75976	0.935	0.040
300.65	-2.9143	0.402386	0.710581	0.753933	-3.88306	0.924	0.042
303.15	-2.8607	0.404500	0.602534	0.635287	-3.68440	0.920	0.042
305.65	-2.8357	0.447719	0.703399	0.460287	-3.70794	0.909	0.044
308.15	-2.8009	0.419910	0.846442	0.497212	-3.99302	0.911	0.043
310.65	-2.7668	0.506900	0.979648	0.264480	-4.25354	0.903	0.045
313.15	-2.8155	0.314628	1.362243	0.300376	-4.81885	0.894	0.043

Table 5- Calculated Partial Excess Molar Volumes at Infinite Dilution at T = (293.15 to 313.15) K from Redlich−Kister Parameters Ai

	Methanol(1) + Water(2)		Ethanol(1) + Water(2)		1-Propanol(1) + Water(2)	
	$\bar{V}_1^{E,\infty}$	$\bar{V}_2^{E,\infty}$	$\bar{V}_1^{E,\infty}$	$\bar{V}_2^{E,\infty}$	$\bar{V}_1^{E,\infty}$	$\bar{V}_2^{E,\infty}$
T(K)	10^6.m^3·mol^{-1}	10^6.m^3·mol^{-1}	10^6.m^3·mol^{-1}	10^6.m^3·mol^{-1}	10^6.m^3·mol^{-1}	10^6.m^3·mol^{-1}
293.15	-2.68863	-4.18731	-4.26567	-3.77069	-7.60614	-4.65946
295.65	-2.77115	-4.11528	-4.38939	-4.06607	-7.49325	-5.10182
298.15	-2.95482	-4.16806	-4.46264	-4.09281	-7.35033	-4.95988
300.65	-3.04215	-4.19048	-4.59058	-4.26957	-7.24306	-4.93042
303.15	-3.12885	-4.37567	-4.66931	-4.22149	-6.98231	-4.90273
305.65	-2.97076	-4.29862	-4.75377	-4.31260	-6.88530	-5.06929
308.15	-3.15211	-4.28593	-4.90446	-4.68856	-6.86458	-5.03033
310.65	-3.14024	-4.46819	-4.97724	-4.51755	-6.81202	-5.26926
313.15	-3.3881	-4.73374	-5.07111	-4.9332	-6.88715	-5.65714

water+methanol, water+ethanol and water+1-propanol binary solvent mixture were compared with calcutated values of V^E by Redlich−Kister [7] type smoothing equation:

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

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

Tables 4. The values of the partial excess volume of solvent$_1$ and solvent$_2$ at infinite dilution $\overline{V}_1^{E,\infty}$ can be calculated as in Table 5 from the adjustable parameters of Redlich−Kister smoothing equation as

$\overline{V}_1^{E,\infty}$=A$_0$-A$_1$+A$_2$-A$_3$+A$_4$ …(3)

$\overline{V}_2^{E,\infty}$= A$_0$+A$_1$+A$_2$+A$_3$+A$_4$ ….(4)

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

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

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 4 indicates good agreement between the calculated and experimental values.

Apparant molar volume (V_Φ)[8-9] of solution of catechol in pure solvents and binary solvent mixture was calculated by using eq.6

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

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

II. EXPERIMENTAL SECTIONS

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

Name of Chemical	Name of supplier	Percentge purity	Standard
Catechol	Sigma-Aldrich co.	≥99%	Reagent Grade
Methanol	Merck, ,Germany.	≥99.8%	G.R.
Ethanol	Merck,D,Germany.	≥99.8%	G.R.
1-Propanol	Spectrochem Mumbai, India.	≥99.8%	HPLC

2 Apparatus and Procedure:-The apparatus and procedures used for density measurement have been described earlier in detail [10-11]. Briefly in this work; an excess amount of catechol 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 long 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 1 hr. 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 of catechol was calculated by constant weights of solute and solvent. This flask solution were used to fill bicapillary pycnometer.

Densities were determined using a 15 cm^3 bicapillary pycnometer as described earlier [12-13]. For calibration of pycnometer triply distilled and degassed water with a density of 0.99705 g·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·m^{-3}.

III. RESULTS AND DISCUSSION

The experimental values of density (ρ) of pure water, methanol, ethanol,1-propanol and water+methanol, water+ethanol,water+1-propanol binary solvents also the densities of the saturated solutions of catechol in water, methanol, ethanol,1-propanol and their binary mixtures water+methanol, water+ethanol,1-propanol have been experimentally measured for comparative studies 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 to values obtained from Redlich−Kister , Apparant molar volume(V_Φ) are given in Table-1,2,3. Calculated Partial Excess Molar Volumes at Infinite Dilution at T

= (293.15 to 313.15) K from Redlich−Kister Parameters Ai shown in Table 5. V^E negative contribution, might arise from following effects

- ✓ Strong interactions between water and alcohol, which enhance the solvent structure in the mixtures.
- ✓ Breaking of intra-molecular hydrogen-bonded structure of one solvent by the addition of other solvent to form intermolecular hydrogen-bond which gives a more compact structure as well as geometrical effects such as interstitial accommodation, making V^E negative.
- ✓ As solute catechol and solvents alcohols, water, their mixture are polar shows dipole-dipole interactions.

The trained for more negative values V^E for all measured temperatures over the entire composition of binary solvent mixture was water+ethanol > water+methanol > water+1-propanol. The highest negative V^E values for water+ethanol , water+methanol and water+1-propanol were observed at 0.3-0.5,0.5 and 0.5 mole fraction of respective binary solvent systems as noticeably shown in Fig.1,2,3 The positive value of V_Φ indicate greater solute-solvent interactions. V_Φ values of Catechol increase with mole fraction and temperture of the system. In water V_Φ values are higher than in pure alcohols. Also noted that positive value of V_Φ for catechol are more in water+1-propanol >water+methanol than >water+ethanol ternary system as shown in Fig.4,5,6.

Computational study using Gaussian 09 software, with DFT, B3LYP, 6-31(G)d method 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 as shown in Fig.7-9, also with catechol molecule as shown in Fig.10-12. 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 catechol was given in Table 6.

IV. IV. CONCLUSION

The data of densities increases as function of concentration .The molality (m) of catechol in pure and binary solvent system were given in Table 1,2,3 .In general the trained of m in binary solvent mixture were shown as water+methanol > water+ethanol > water+1-propanol. But it should be notice that initial mole fraction(0.1,0.2,0.3) of water+1-propanol and water+ethanol molality values was observed to be higher than water+methanol system which was exactly reverse than that of general trained. This reverse trained, water+1-propanol > water+ethanol > water+methanol was observed in case of apparent molar volume (V_Φ) in all mole fractions solvent system which was against the rule "like dissolved like". Further V_Φ valves increase with increase of temperature. In Table 6 dipole moment obtained from DFT of catechol+alcohol in solvent phase water was observed to be decreasing as catechol+1propanol > catechol +ethanol > catechol +methanol.

V. ACKNOWLEDGMENTS

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Table 6- Theoretical data obtained by Gaussian 09 by DFT, B3LYP , 6-31(G)d method.

Molecule	Phase	Dipole Moment (Debye)	Total Energy(a.u.)	Symmetry Point group	Alcoholic (-OH) Freq.cm^{-1}	Alcoholic (-OH) Bond Distance(^{0}A)	H-Bonding Distance(A0) in Alcohol & Water
Methanol	Gas	1.6942	-115.71441	C2V	3609.22	0.968744	-
	Water	1.9739	-115.71943	C2V	3606.66	0.969642	-
Ethanol	Gas	1.5613	-115.03380	CS	3607.31	0.969031	-

	Water	1.9063	-115.03856	CS	3601.80	0.970082	-
1-Propanol	Gas	1.488	-194.34750	C1	3608.16	0.968948	-
	Water	1.8451	-194.35226	C1	3602.54	0.969942	-
Methanol+H_2O	Gas	2.2338	-192.13567	C1	3391.18	0.976877	1.903509
	Water	3.4643	-192.14679	C1	3477.48	0.982090	1.832844
Ethanol+H_2O	Gas	2.2392	-231.45914	C1	3469.99	0.977556	1.905407
	Water	3.4239	-231.46581	C1	3381.81	0.982355	1.835451
1-Propanol+H_2O	Gas	2.2959	-270.76864	C1	3473.21	0.977224	1.903446
	Water	3.3881	-270.77954	C1	3381.89	0.982300	1.834326
Methanol+ Catechol	Gas	3.5145	-458.41185	C1	3537.34	0.974753	1.916591
	Water	4.8952	-458.42285	C1	3522.66	0.975807	1.947404
Ethanol+ Catechol	Gas	3.5486	-537.73150	C1	3532.16	0.975263	1.928707
	Water	4.9847	-537.74239	C1	3519.85	0.976205	1.953120
1-Propanol+ Catechol	Gas	3.5209	-577.04548	C1	3530.01	0.975412	1.929670
	Water	5.0179	-577.056206	C1	3520.84	0.976140	1.959044

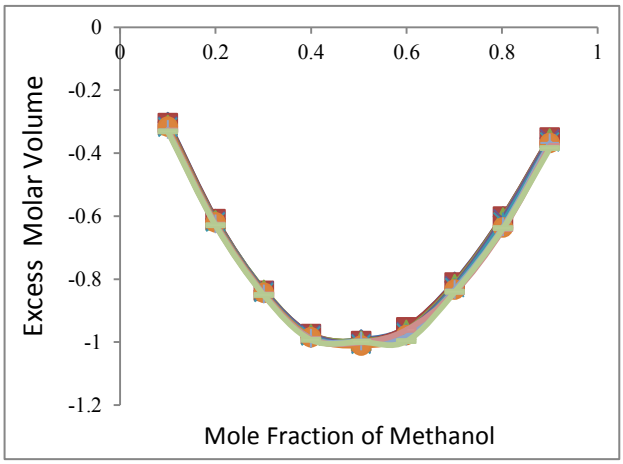

Fig.1- Graph for Excess molar volumes (V^E) vs. Mole fraction of water+methanol binary system.

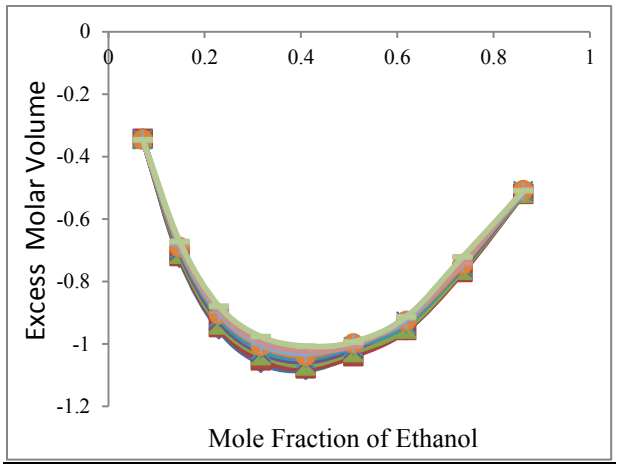

Fig.2- Graph for Excess molar volumes (V^E) vs. Mole fraction of water+ethanol binary system.

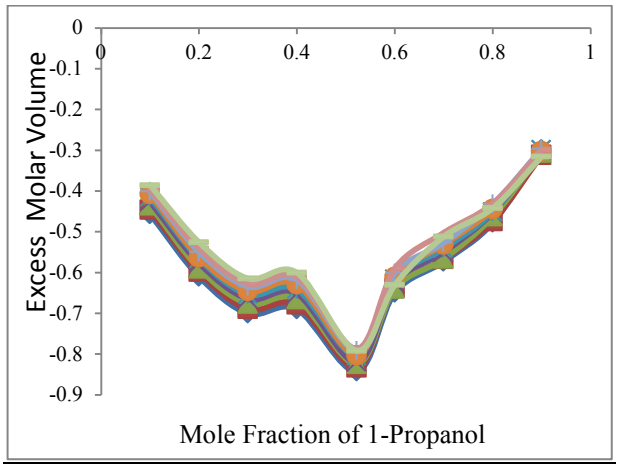

Fig.3- Graph for Excess molar volumes (V^E) vs. Mole fraction of water+1-propanol binary system.

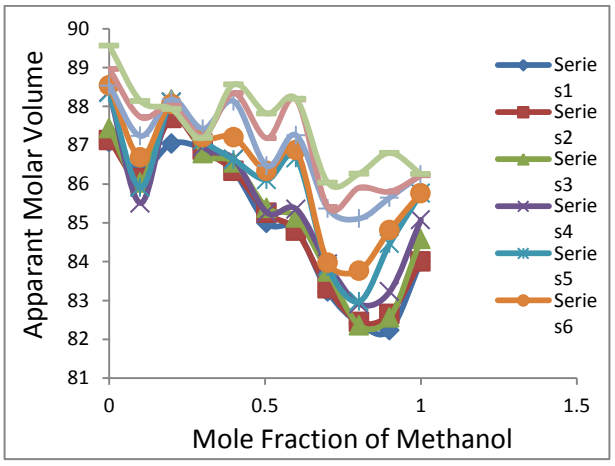

Fig.4- Graph of Apparant molar volume (V_Φ) of Catechol vs. Mole fraction of water+methanol binary system..

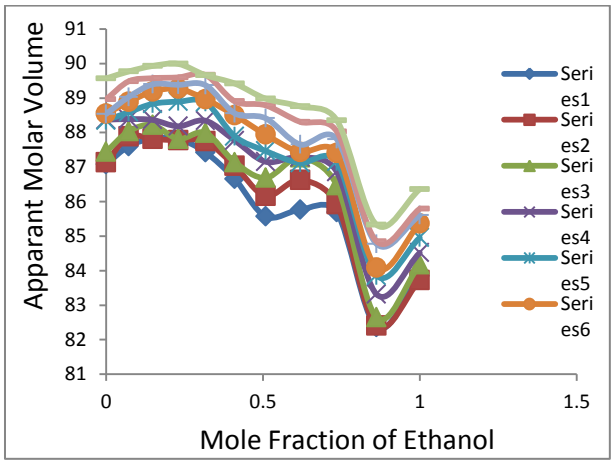

Fig.5- Graph of Apparant molar volume (V_Φ) of Catechol vs. Mole fraction of water+ethanol binary system.

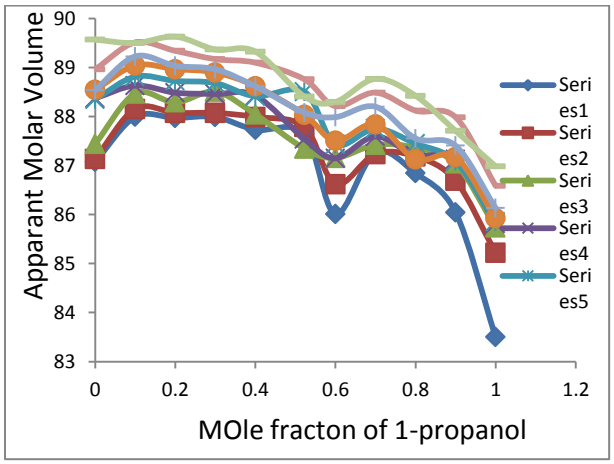

Fig.6- Graph of Apparant molar volume (V_Φ) of Catechol vs. Mole fraction of water+1-propanol binary system.

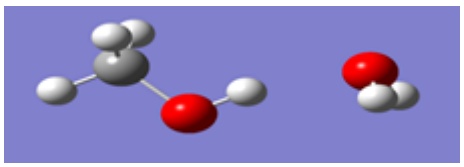

Fig.7-Optimized structure of Methanol+Water

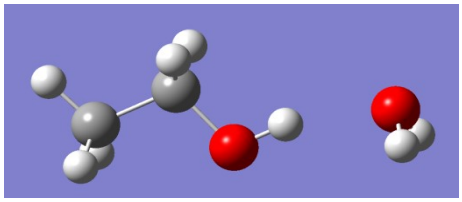

Fig.8-Optimized structure of Ethanol+Water

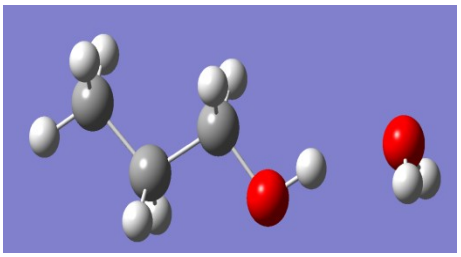

Fig.9-Optimized structure of 1-Propanol+Water

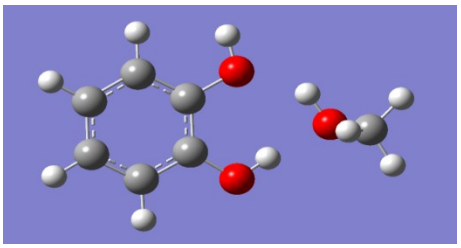

Fig.10-Optimized structure of Catechol+Methanol

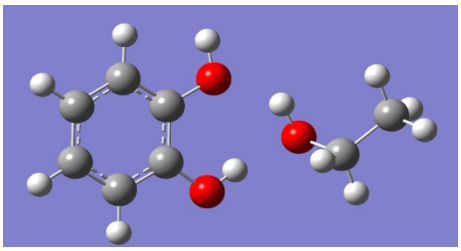

Fig.11-Optimized structure of Catechol+Ethanol

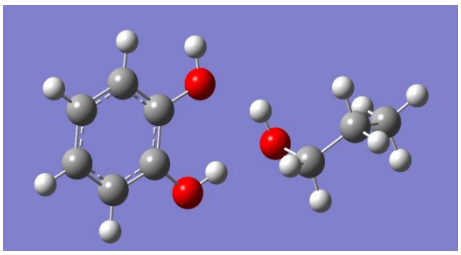

Fig.12-Optimized structure of Catechol+1-Propanol

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