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Solubility of Phenolic Compounds in Pure Water and Alcohols with FTIR and DFT Study

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ABSTRACT

Solubility studies are significant from the point of view of understanding the science of solution. The solubility of solute in solvent depends upon the nature of solute and solvent. Also depend upon operating temperature, pressure of the system. Mole fraction solubility (x_B) of studied phenolic compounds were determined at (293.15, 298.15, 303.15 & 308.15) K. FTIR spectra were recorded for pure solvents and binary solutions prepared by dissolving phenolic compound in same solvents at room temperature. For structural variation, biological activity and industrial importance we select catechol, hydroquinone and 2-naphthol as studied phenolic compounds. Spectral data used to determine various molecular interactions. Theoretical study of experimental molecules and their combinations were optimized on Window-7, Intel core i5 system. 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.

Keyword: Solubility, Catechol, Hydroquinone, 2-Naphthol, FTIR, DFT.

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 interactions between molecules. 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 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.[5] Several naphthalene containing drugs are available, such as nafacillin, naftifine, tolnaftate, terbinafine etc. which play vital role in the control of microbial infection. Several other synthetic derivatives have also been reported which possess significant and satisfactory antimicrobial property. β-naphthol commonly used as dye possess a very good antimicrobial property[6].

Solvent-solvent and solvent-solute interactions of electrolytes are extremely important for the synthesis, design of processes and simulations of unit operations [7]. The experimental work was carried out at (293.15 to 308.15) K and solubilities were calculated gravimetrically shown in Table 1 using eq.1.

$$x_B = [mB/MB]/[mA/MA + mB/MB] \quad \text{……..(1)}$$

Where x_B is mole fraction solubility of solute, B is solute used, A is solvent used, m is mass in grams and M represent the molecular weight, the density and the molecular weight.

Table 1- Mole fraction solubility (x_B) of different solutes in different solvents at various temperatures

Solvent	Solute	Mole fraction solubility (x_B) at various temperatures.			
		293.15 K	298.15 K	303.15 K	308.15 K
Water	Catechol	0.0752	0.1036	0.1445	0.1781
	Hydroquinone	0.0102	0.0122	0.0147	0.0180
	2-Naphthol	0.0000	0.0001	0.0001	0.0001
Methanol	Catechol	0.3484	0.3632	0.3908	0.4097
	Hydroquinone	0.1331	0.1392	0.1458	0.1556
	2-Naphthol	0.2187	0.2319	0.2497	0.2706
Ethanol	Catechol	0.3566	0.3712	0.3917	0.4136
	Hydroquinone	0.1877	0.1964	0.2034	0.2109
	2-Naphthol	0.2487	0.2771	0.2854	0.3040
1-Propanol	Catechol	0.3355	0.3666	0.3823	0.3980
	Hydroquinone	0.1702	0.1791	0.1871	0.1955
	2-Naphthol	0.2332	0.2547	0.2744	0.2960

The HOMO-LUMO energy gap is calculated by equation:

Energy Gap = E. LUMO - E. HOMO …..(2)

Where E. LUMO is energy of LUMO in eV and E. HOMO is energy of LUMO in eV.

Electrochemical properties: E_{HOMO} describes the charge density i.e. higher the E_{HOMO} energy the greater the ability of the molecule to donate electrons. Large $E_{HOMO\text{-}LUMO}$ energy difference means electronic excitation required high energy i.e. electron have less tendency to move to the excited state and such molecules are chemically more inert. [8, 9]

According to Koopman's theorem, global reactivity descriptor such as:

Electronegativity (χ) = -1/2 (E_{HOMO} + E_{LUMO})

Chemical ptantial (μ) = 1/2 (E_{HOMO} + E_{LUMO})

Global hardness (η) = 1/2 (E_{LUMO} - E_{HOMO})

Electrophilicity index (ω) = μ^2 / 2η

Ionization energy (I) = - E_{LUMO}

Electron affinity (A) = - E_{HOMO}

All these values are summarised in Table-5.

II. EXPERIMENTAL SECTIONS

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

Name of Chemical	Name of supplier	Percentage purity	Standard
Catechol	Sigma-Aldrich co.	≥99%	Reagent Grade
Hydroquinone	Sigma-Aldrich co.	99%	Reagent Grade
2-Naphthol	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 solubility measurement have been described earlier in detail [10-14]. Briefly in this work; an excess amount of solute as 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. Solubility of phenolic compounds was calculated by constant weights of solute and solvent.

2.3 FTIR spectra

FTIR spectra of pure solvents and binary solution of solutes in same solvents were study at room temperature. Shimadzu IR affinity-1s is compact FTIR spectrophotometer is used for spectral analysis. Spectral data particularly the change in υ-OH used to determine solvent-solvent and solute-solvent type of interactions in terms of hydrogen bonding [15, 16].

Theoretical study of experimental molecules and their combinations were optimized on Window-7, Intel core i5 system. 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.

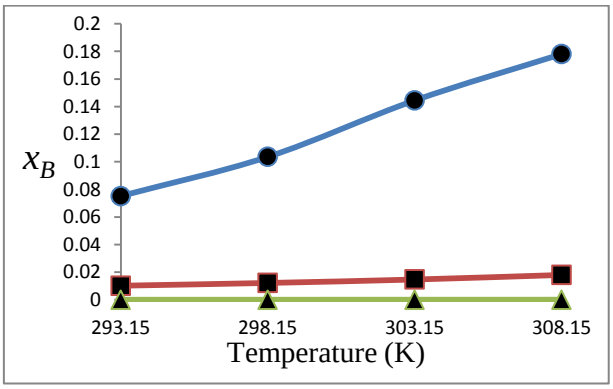


Fig 1. Graph for Mole fraction solubility (x_B) vs. Temperature (K) in Water. (●=Catechol ; ■=Hydroquinone; ▲=2-Naphthol)

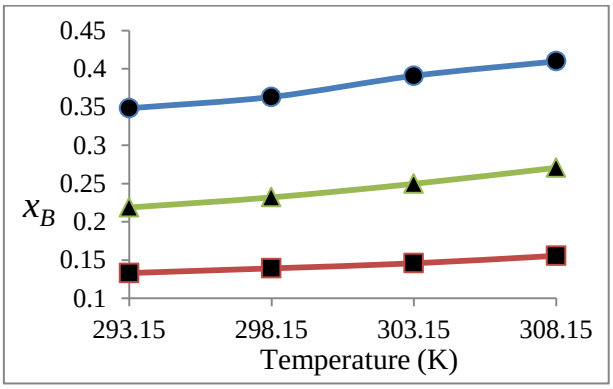


Fig.2- Graph for Mole fraction solubility (x_B) vs. Temperature (K) in Methanol. (●=Catechol ; ■=Hydroquinone; ▲=2-Naphthol)

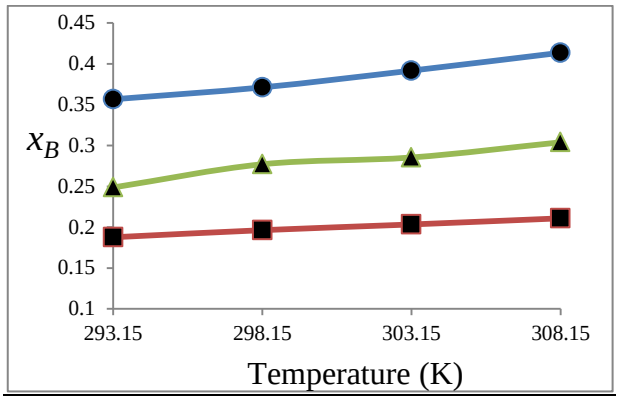


Fig.3- Graph for Mole fraction solubility (x_B) vs. Temperature (K) in Ethanol. (●=Catechol ; ■=Hydroquinone; ▲=2-Naphthol)

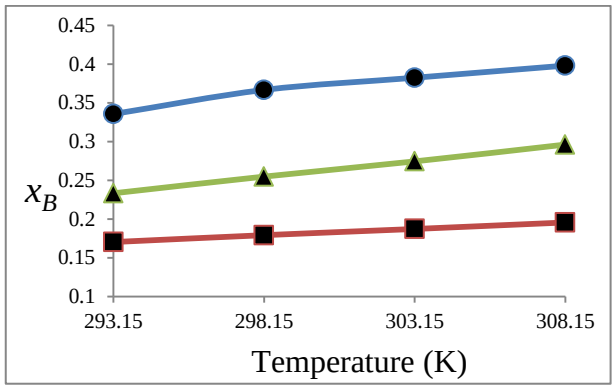


Fig.4- Graph for Mole fraction solubility (x_B) vs. Temperature (K) in 2-Propanol. (●=Catechol ; ■=Hydroquinone; ▲=2-Naphthol)

Table 2- Experimental υ-OH for 0, 0.2, 0.5, 0.7 and 1 mole fraction of alcohol (x_c^0) in binary and ternary solutions.

Solute	Solvent	Experimental υ-OH alcohol cm^{-1}	Experimental υ-OH Solute+Solvent cm^{-1}
Catechol	Water	-	3394.72
	Methanol	3347	3360
	Ethanol	3358	3332.99
	1-Propanol	3340	3332.99
Hydroquinone	Water	-	3387
	Methanol	3347	3332.99
	Ethanol	3358	3332.99
	1-Propanol	3340	3329.14
2-Naphthol	Water	-	3383.14
	Methanol	3347	3332.99
	Ethanol	3358	3336.85
	1-Propanol	3340	3336.85

Table 3-HOMO, LUMO energies and Energy Gap between LUMO-HOMO Calculated by DFT method at B3LYP level (d) using 6-31G basis set.

System	Phase/Media	HOMO (eV)	LUMO (eV)	LUMO-HOMO Energy gap (eV)
C	Gas	-5.624	0.219	5.843
	Water	-8.179	-4.047	4.132
H	Gas	-5.412	-0.062	5.350
	Water	-5.536	-0.174	5.361
N	Gas	-5.517	-0.922	4.595
	Water	-5.665	-1.054	4.611
W	Gas	-7.924	1.704	9.628
	Water	-8.035	2.062	10.097
M	Gas	-7.198	2.047	9.246
	Water	-7.281	2.283	9.564
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
WC	Gas	-5.540	0.235	5.775
	Water	-5.695	0.114	5.809
MC	Gas	-5.539	0.247	5.787
	Water	-5.703	0.109	5.812
EC	Gas	-5.520	0.258	5.778
	Water	-5.692	0.111	5.803
PC	Gas	-5.527	0.250	5.776
	Water	-5.688	0.113	5.801
WH	Gas	-4.926	0.365	5.290
	Water	-5.316	-0.036	5.280
MH	Gas	-4.914	0.370	5.283
	Water	-5.321	-0.039	5.282
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
WN	Gas	-5.103	-0.561	4.542
	Water	-5.486	-0.939	4.547
MN	Gas	-5.095	-0.558	4.537
	Water	-5.490	-0.941	4.549
EN	Gas	-5.078	-0.543	4.535
	Water	-5.489	-0.940	4.549
PN	Gas	-5.080	-0.546	4.535
	Water	-5.491	-0.941	4.550

Table 4- Theoretical Thermodynamic functions calculated by DFT/B3LYP method at 6-31G (d) basis set

Molecule	Phase/ Media	E (RB3LYP) a.u.	Zero point vibrational energy Kcal/mol.	Nuclear Repulsion Energy Hartrees	Total Energy(a.u.)		
					E(Thermal) Kcal/mol.	C_v cal/mol.Kelv.	S cal/mol.Kelv.
C	Gas	-382.68162	68.29475	350.698	72.536	26.54	80.44
	Water	-382.68967	68.16156	350.5293	72.399	26.57	80.39
H	Gas	-382.678	68.1481	343.8718	72.406	26.712	80.57
	Water	-382.688	67.9844	343.6457	72.251	26.775	80.631
N	Gas	-461.10832	95.18956	543.2950	100.24	33.587	87.634
	Water	-461.11604	95.20691	542.9885	100.25	33.537	87.591
W	Gas	-76.40895	13.2834	9.088237	15.062	5.997	45.14
	Water	-76.41630	13.25463	9.079528	15.033	5.997	45.15
M	Gas	-115.71441	32..29795	40.21749	34.364	8.668	56.74
	Water	-115.71943	32.24812	40.15408	34.326	8.72	56.82
E	Gas	-115.03380	50.39846	81.60958	53.074	13.377	64.95
	Water	-115.03856	50.29175	81.49033	52.985	13.454	64.47
P	Gas	-194.34750	68.41857	130.046	71.887	18.226	72.05
	Water	-194.35226	68.27776	129.9444	71.772	18.313	72.26
WC	Gas	-459.10680	83.88594	438.1257	89.974	35.759	99.51
	Water	-459.12005	83.69986	438.7085	89.709	35.738	95.65
MC	Gas	-458.41185	102.3131	521.1904	109.24	39.146	106.22
	Water	-458.42285	102.0336	520.0871	108.95	39.280	105.30
EC	Gas	-537.73150	120.2570	604.2595	127.93	43.943	115.11
	Water	-537.74239	119.9584	603.6739	127.64	44.032	114.49
PC	Gas	-577.04548	138.2846	690.7837	146.76	48.687	121.52
	Water	-577.05621	137.9132	689.0442	146.41	48.806	122.72
WH	Gas	-459.102	83.3329	421.6249	89.842	36.817	100.96
	Water	-459.119	83.3464	423.0705	89.662	36.467	98.159
MH	Gas	-498.408	101.8813	498.5584	109.12	39.960	110.63
	Water	-498.422	101.7442	498.7914	108.90	39.857	108.50
EH	Gas	-537.728	119.9227	576.0097	127.84	44.663	117.56
	Water	-537.741	119.7989	576.4233	127.65	44.457	116.96

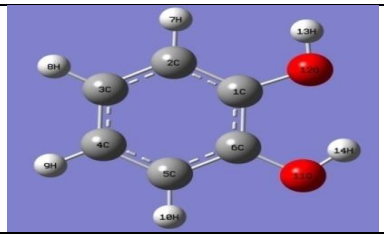
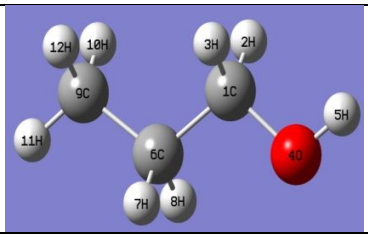
PH	Gas	-577.041	137.9155	654.7609	146.67	49.518	125.63
	Water	-577.055	137.7685	655.6081	146.43	49.370	122.53
WN	Gas	-537.53323	110.31542	632.6690	117.64	43.706	108.38
	Water	-537.54727	110.44335	634.2467	117.54	43.275	104.71
MN	Gas	-576.83842	128.9223	717.9539	136.96	46.803	117.40
	Water	-576.84997	128.8124	718.6284	136.78	46.656	116.21
EN	Gas	-616.15844	146.9624	801.6599	155.67	51.516	123.46
	Water	-616.16976	146.8245	803.3674	155.48	51.352	122.46
PN	Gas	-655.47232	165.0252	891.7256	174.54	56.322	130.13
	Water	-655.48354	164.8245	889.2642	174.30	56.215	129.47

Table 5- Global chemical reactivity indices.
[Chemical Hardness (Ƞ), Chemical Softness (б), Electronegativity (χ), Electrochemical potential (μ), Global electrophilicity index (ω), Electron affinity (A), Ionization energy (I)]

Molecule	Phase/ Media	Ƞ (eV)	б (eV)	χ (eV)	μ (eV)	ω (eV)	A (eV)	I (eV)
C	Gas	2.92	0.34	2.70	-2.70	1.25	-0.22	5.62
	Water	2.07	0.48	6.11	-6.11	9.04	4.05	8.18
H	Gas	2.68	0.37	2.74	-2.74	1.40	0.06	5.41
	Water	2.68	0.37	2.86	-2.86	1.52	0.17	5.54
N	Gas	2.30	0.44	3.22	-3.22	2.26	0.92	5.52
	Water	2.31	0.43	3.36	-3.36	2.45	1.05	5.66
W	Gas	4.81	0.21	3.11	-3.11	1.00	-1.70	7.92
	Water	5.05	0.20	2.99	-2.99	0.88	-2.06	8.04
M	Gas	4.62	0.22	2.58	-2.58	0.72	-2.05	7.20
	Water	4.78	0.21	2.50	-2.50	0.65	-2.28	7.28
E	Gas	4.60	0.22	2.52	-2.52	0.69	-2.08	7.12
	Water	4.75	0.21	2.45	-2.45	0.63	-2.30	7.20

P	Gas	4.61	0.22	2.50	-2.50	0.68	-2.11	7.11
	Water	4.77	0.21	2.44	-2.44	0.62	-2.33	7.21
WC	Gas	2.89	0.35	2.65	-2.65	1.22	-0.23	5.54
	Water	2.90	0.34	2.79	-2.79	1.34	-0.11	5.70
MC	Gas	2.89	0.35	2.65	-2.65	1.21	-0.25	5.54
	Water	2.91	0.34	2.80	-2.80	1.35	-0.11	5.70
EC	Gas	2.89	0.35	2.63	-2.63	1.20	-0.26	5.52
	Water	2.90	0.34	2.79	-2.79	1.34	-0.11	5.69
PC	Gas	2.89	0.35	2.64	-2.64	1.21	-0.25	5.53
	Water	2.90	0.34	2.79	-2.79	1.34	-0.11	5.69
WH	Gas	2.65	0.38	2.28	-2.28	0.98	-0.36	4.93
	Water	2.64	0.38	2.68	-2.68	1.36	0.04	5.32
MH	Gas	2.64	0.38	2.27	-2.27	0.98	-0.37	4.91
	Water	2.64	0.38	2.68	-2.68	1.36	0.04	5.32
EH	Gas	2.64	0.38	2.26	-2.26	0.97	-0.38	4.90
	Water	2.64	0.38	2.68	-2.68	1.36	0.04	5.32
PH	Gas	2.64	0.38	2.25	-2.25	0.96	-0.39	4.89
	Water	2.64	0.38	2.68	-2.68	1.36	0.04	5.32
WN	Gas	2.27	0.44	2.83	-2.83	1.77	0.56	5.10
	Water	2.27	0.44	3.21	-3.21	2.27	0.94	5.49
MN	Gas	2.27	0.44	2.83	-2.83	1.76	0.56	5.09
	Water	2.27	0.44	3.22	-3.22	2.27	0.94	5.49
EN	Gas	2.27	0.44	2.81	-2.81	1.74	0.54	5.08
	Water	2.27	0.44	3.21	-3.21	2.27	0.94	5.49
PN	Gas	2.27	0.44	2.81	-2.81	1.74	0.55	5.08
	Water	2.28	0.44	3.22	-3.22	2.27	0.94	5.49

Fig. 5-Optimized structures of solute, solvents combinations by DFT method at B3LYP level using 6-31G(d) basis set.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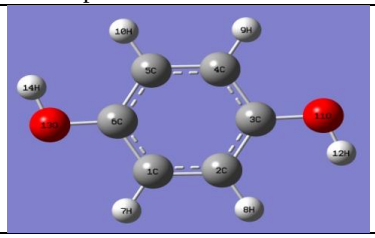	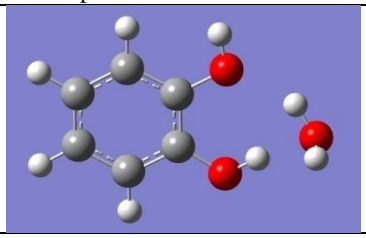
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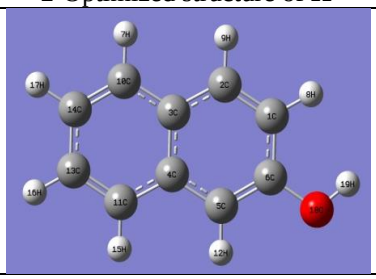	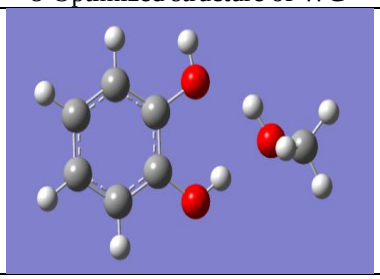
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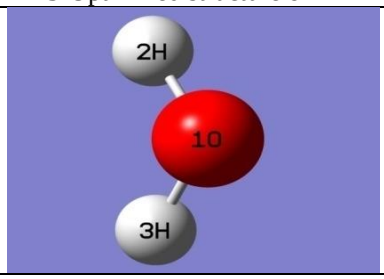	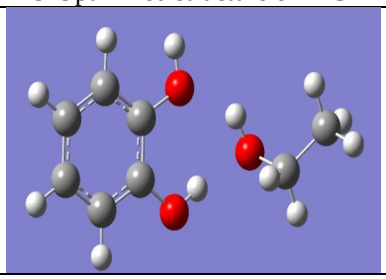
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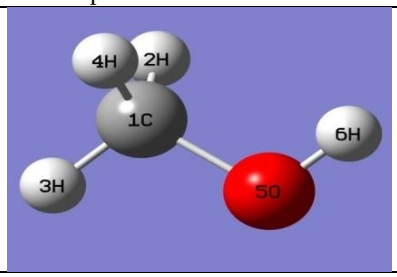	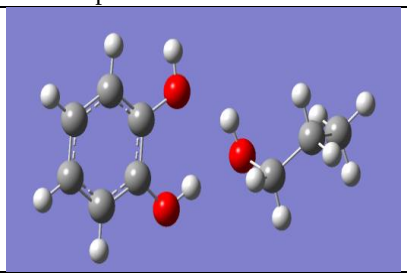
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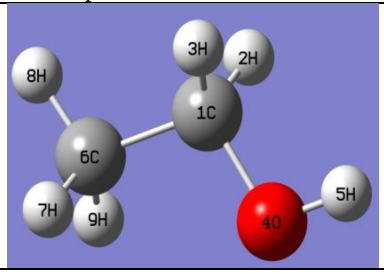	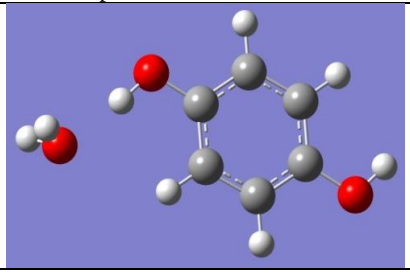
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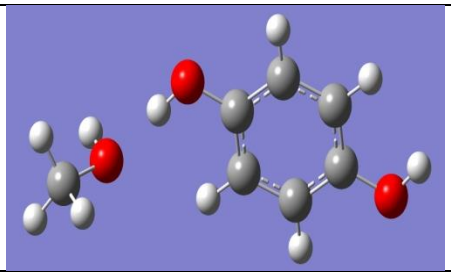	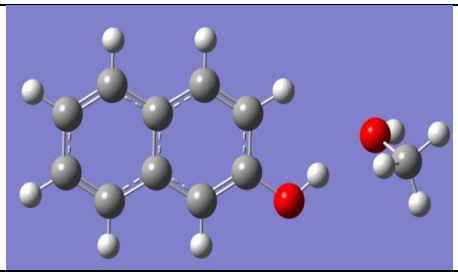
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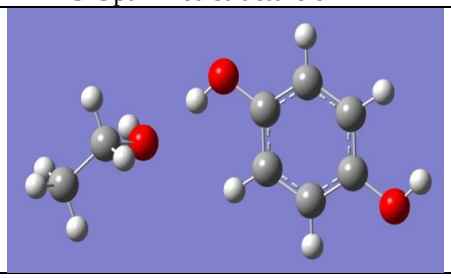	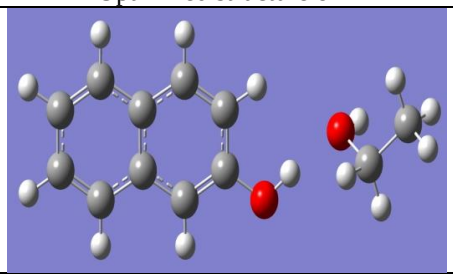
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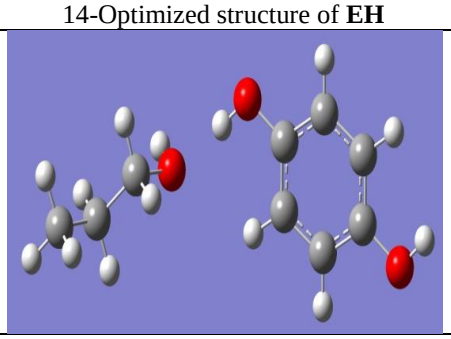	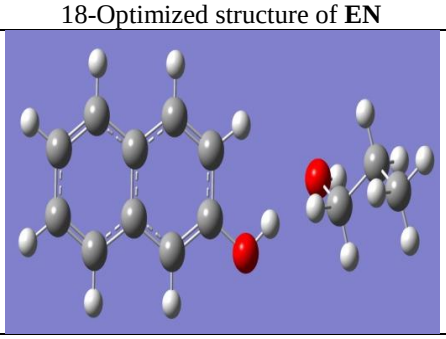
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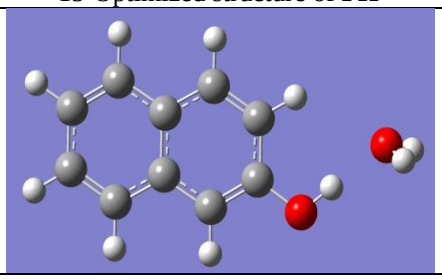
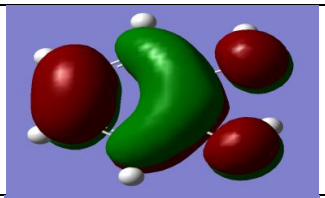
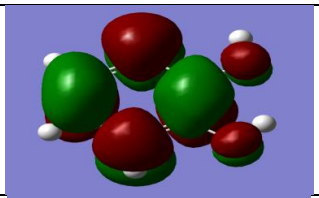
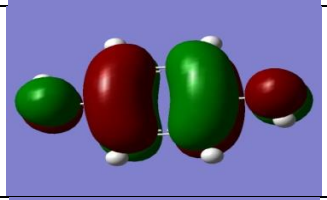
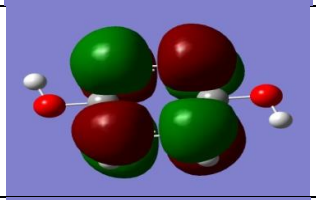
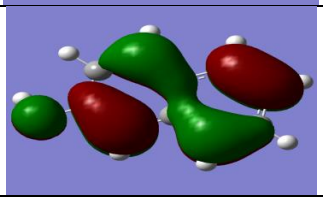
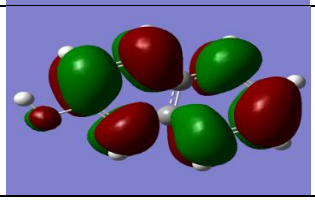
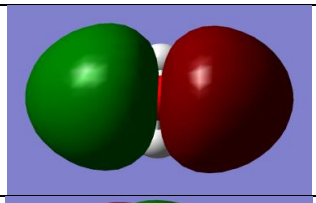
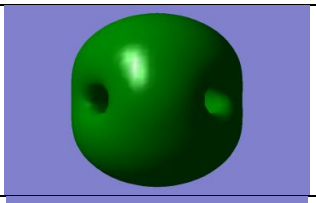
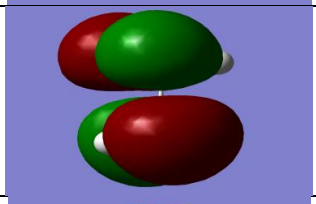
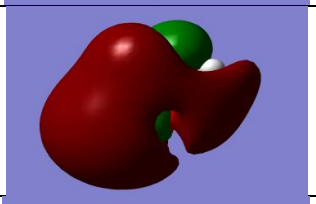
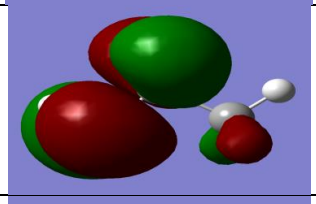
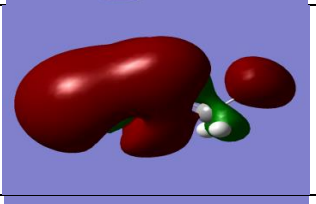
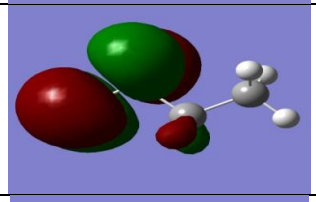
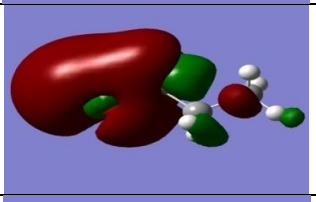
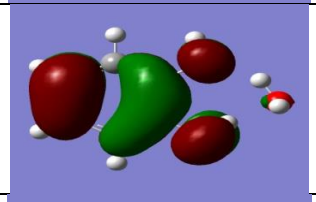
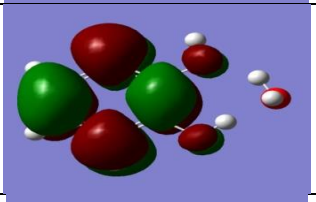
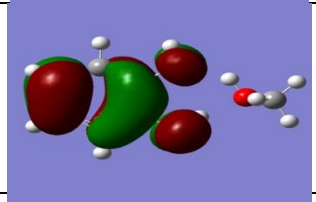
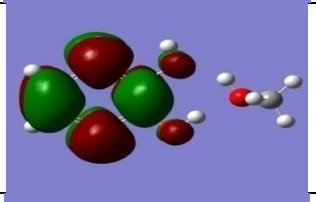
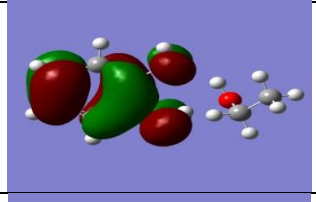
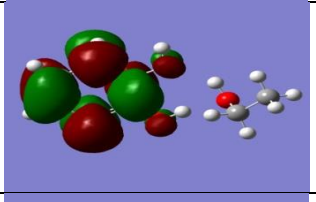
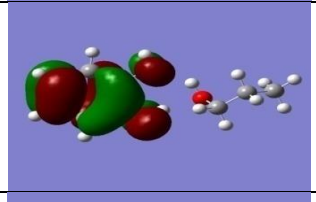
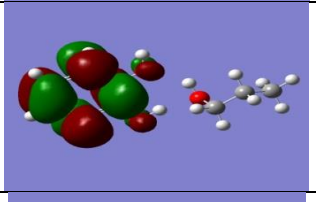
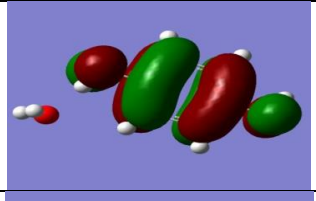
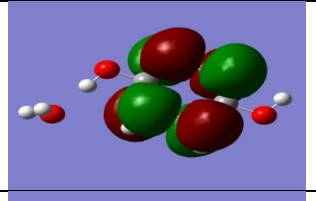
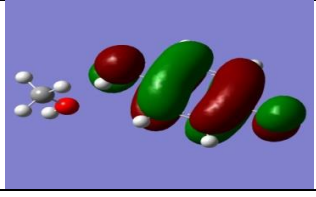
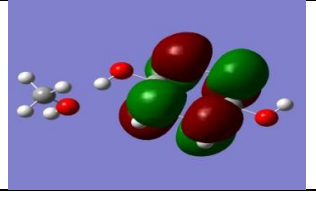
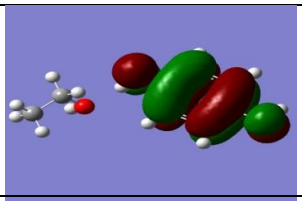
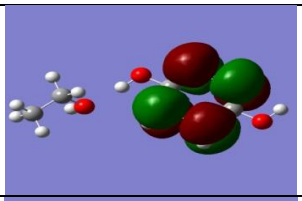
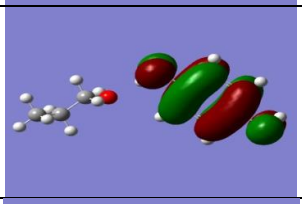
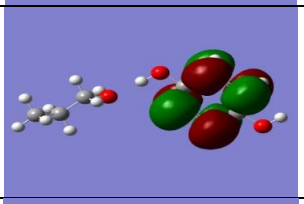
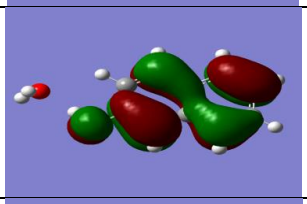
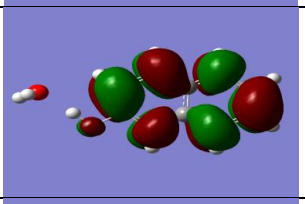
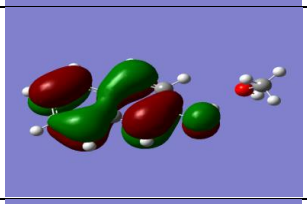
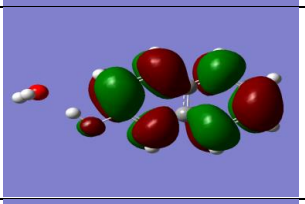
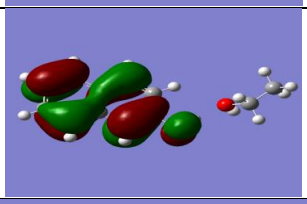
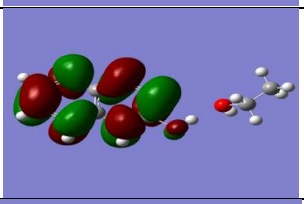
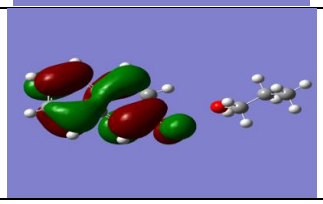
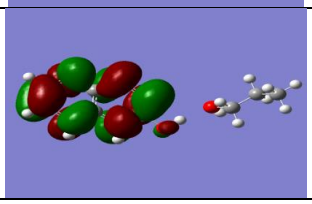
	
16-Optimized structure of **WN**	

Fig. 6-HOMO, LUMO structures with LUMO-HOMO Energy Gap.

Molecule	HOMO	L-H E.G.(eV)	LUMO
C		Gas 5.843	
		Water 4.132	
H		Gas 5.350	
		Water 5.361	
N		Gas 4.595	
		Water 4.611	

W		Gas 9.628 Water 10.097		
M		Gas 9.246 Water 9.564		
E		Gas 9.202 Water 9.505		
P		Gas 9.227 Water 9.538		
WC		Gas 5.775 Water 5.809		
MC		Gas 5.787 Water 5.812		
EC		Gas 5.778 Water 5.803		
PC		Gas 5.776 Water 5.801		
WH		Gas 5.290 Water 5.280		
MH		Gas 5.283 Water 5.282		

EH		Gas 5.281 Water 5.282	
PH		Gas 5.281 Water 5.283	
WN		Gas 4.542 Water 4.547	
MN		Gas 4.537 Water 4.549	
EN		Gas 4.535 Water 4.549	
PN		Gas 4.535 Water 4.550	

II. RESULTS AND DISCUSSION

At same temperature the solubility trend of catechol in pure solvent was ethanol > methanol > 1-propanol > water. At same temperature the solubility trend of hydroquinone in pure solvent was ethanol > 1-propanol > methanol > water. At same temperature the solubility trend of 2-naphthol in pure solvent was ethanol > 1-propanol > methanol > water. This was clearly seen from Table-1 and Fig. 1,2,3,4 at temperatures (293.15, 298.15, 303.15 & 308.15) K.

FTIR data given in Table-2, indicate that for alcoholic solvent the trend of decreasing υ-OH is ethanol > methanol > 1-propanol. Suggested that ethanol shows less interaction among them so more free to interacts with solute and thus we observed that all three solute have most solubility in ethanol than methanol and 1-propanol. Again water solution of three phenols have very high υ-OH, showing weak interaction between water and phenolic solute, hence less solubility than the alcoholic solutions. As the change length of alcohol increase υ-OH of solution decreases indicating after ethanol solubility is more in 1-propanol than in methanol. But in case of catechol solubility was more in methanol than in 1-propanol this is because of catechol has two intra-molecular hydrogen bonded –OH groups and others hydroquinone, 2-naphthol have free –OH group.

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 and water then interacted with solute molecule

as shown in Fig.5. Total energy, heat capacity at constant volume, entropy, zero-point vibrational energy and nuclear repulsion energy are given in Table 4.

III. CONCLUSION

In general from Fig. 2, 3, 4, the solubility trend of different solute in pure alcohols was catechol > 2-Naphthol > Hydroquinone. This was explain on the basis of HOMO-LUMO energy gap, the decreasing trend of energy gap for solutions of solute in all four solvents was catechol > 2-Naphthol > Hydroquinone , as shown in Table-3 and Fig. 6. But in pure water solubility of hydroquinone was more than the 2-Naphthol. The decreasing trend of solubility in water was catechol > Hydroquinone > 2-Naphthol, which was explain on the basis size of solute as size of solute increase, solubility decrease. Thermochemical parameters as given in Table-4, shows increasing trend of all these parameter from top to bottom for each series like series of solutes(C>H>N), series of solvents(W>M>E>P) and series of different solute in binary solutions(WC>MC>EC>PC similarly for/H/N systems) These thermochemical parameters are total energy, heat capacity at constant volume, entropy, zero-point vibrational energy and nuclear repulsion energy can provide valuable information about these molecules for further study when these compounds consider as starting materials in new reactions.

IV. ACKNOWLEDGMENTS

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V. REFERENCES

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