DFT Study of Catechol Molecule and Catechol With Different Solvent Systems

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Abstract: Theoretical study using Gaussian 03 software, with DFT/ B3LYP method at 6-31G(d) basis set was performed to understand the fundamental interactions between solvent-solvent and catechol-solvent molecules and data obtained is used for guide line for overall stability of catechol in different solvents. Computational study of Catechol, catechol+water, Catechol+methanol and catechol+methanol+water systems are found to be useful to get the HOMO, LUMO, thermodynamic properties HOMO-LUMO energy gap used to calculate global chemical reactivity indices by using Koopmans theorem.

Keywords: DFT, HOMO-LUMO, Catechol, Koopmans theorem.

I. INTRODUCTION

A range of catechol-rich foodstuffs, ranging from beverages to fruit and vegetable extracts, along with the purified preparations of commonly consumed dietary catechols to modulate the growth of enteropathogenic bacteria[1]. Ismail Kocacaliskan et al. [2] reported antimicrobial activity of catechol against selected bacteria.B. Gigante et al. [3] synthesized catechol derivative, possess variour biological activity such as antiviral, antifungal, antitumor. One of catechol derivative 11,12-dihydroxyabietate-8,11,13-trien-15-oate (2) having an dehydroabietane skeleton. Its properties were compared with carnosic acid, a naturally occurring catechol with same skeleton structure possess antioxidant anticancer and antiviral properties. Further reported that synthesised catechol derivative (2) showed better activity than natural catechol derivative. Hence we select catechol for your study. These data is useful to the field of solution chemistry and organic synthesis

II. EXPERIMENTAL:

COMPUTATIONAL DETAILS:

In this study Catechol, Methanol, Water are experimental molecules and their combinations were optimized on Window-7, Intel core i7 with 16 GB RAM of system. Computational study using Gaussian 03W software, DFT/ B3LYP method, 6-31(G)d as basis set was performed to understand the fundamental interactions between solvent-solvent and solute-solvent molecules. Theoretical study helps to understand the stability and orientation of molecular systems.

According to Koopmans theorem [4], global reactivity descriptor such as:

- Electronegativity (χ): It is the attracting power of an atom in a molecule. Higher is the electronegativity, greater its electron accepting power. It is calculated as

$$(\chi) = -1/2\ (E_{HOMO} + E_{LUMO}) \quad \text{--- (1)}$$

- Chemical potential (μ): It is the negative value of electronegativity of a molecule. It is also calculated as half of the sum of HOMO and LUMO energy as given below

$$(\mu) = 1/2\ (E_{HOMO} + E_{LUMO}) \text{ or } \mu = -\chi \quad \text{--- (2)}$$

- Chemical Hardness (Η) and Chemical Softness (б): Chemical hardness is related with the electronic excitation or charge transfer. It gives the stability and reactivity of chemical system.[5] It is calculated as

$$(\Eta) = 1/2\ (E_{LUMO} - E_{HOM} \quad \text{--- (3)}$$

Chemical Softness is reciprocal of global hardness[6-8], calculated as follow

$$(б) = 1 / \Eta \quad \text{--- (4)}$$

- Electrophilicity index (ω)[14]: It is the ability or capacity of a chemical species to accommodate additional electronic charge from its surrounding and stabilization of its energy state. It is calculated as;

$$(\omega) = \mu^2 / 2\Eta \quad \text{--- (5)}$$

- Ionization energy (I) and Electron affinity (A): According to Koopmans theorem ionization energy and electron affinity are approximated as the negative values of the HOMO and LUMO energies respectively. They are obtained as;

$$(I) = -E_{LUMO} \quad \text{--- (6)}$$

$$(A) = -E_{HOMO} \quad \text{--- (7)}$$

III. RESULTS AND DISCUSSIONS

Computational Study*:*

3.1 Mulliken Atomic Charges

Mulliken atomic charges are important tool in the application of quantum chemical calculation to the molecular system. Dipole moments, molecular polarizability and electronic structure of molecular systems is depends on these charges. The calculated Mulliken atomic charges are listed in Table-1,3,5 and atoms are shown in Fig. 1,2,3. The atoms show negative charges which act as donor atom and atoms shows positive charges which act as the acceptor atom[15].

3.2 Optimized Parameters

Bond length(R), bond angle(A) and dihedral angle(D) are the optimized parameters obtained from optimized structure of catechol, solvent and catechol-solvent systems. From Table-2,4,6 gives R, A, D values, which gives importance information of catechol and catechol-solvent interations.

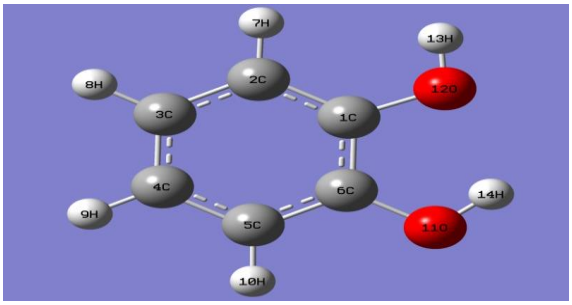


Fig.1 Optimized structure of Catechol

Table-1. Mulliken atomic charges of Catechol

Atom no.	Atom	Charges
1	C	0.29769
2	C	-0.1924
3	C	-0.1415
4	C	-0.1377
5	C	-0.1721
6	C	0.32295
7	H	0.11888
8	H	0.12647
9	H	0.12737
10	H	0.13944
11	O	-0.653
12	O	-0.6792
13	H	0.41644
14	H	0.42677

Table-2. Optimized Parameters of Catechol

Optimized Parameters (Distance in Angstroms and Angle in Degrees)			
Number	Atoms	Å / degree	
		In water	In Methanol
R1	R(1,2)	1.390	1.392
R2	R(1,6)	1.406	1.407
R3	R(1,12)	1.380	1.377
R4	R(2,3)	1.399	1.401
R5	R(2,7)	1.089	1.088
R6	R(3,4)	1.394	1.395
R7	R(3,8)	1.086	1.086
R8	R(4,5)	1.398	1.399
R9	R(4,9)	1.086	1.086
R10	R(5,6)	1.392	1.393
R11	R(5,10)	1.086	1.086
R12	R(6,11)	1.365	1.367
R13	R(11,14)	0.973	0.974
R14	R(12,13)	0.969	0.970
A1	A(2,1,6)	120.514	120.378
A2	A(2,1,12)	124.651	124.830
A3	A(6,1,12)	114.835	114.793
A4	A(1,2,3)	119.792	119.770
A5	A(1,2,7)	119.668	119.620
A6	A(3,2,7)	120.541	120.610
A7	A(2,3,4)	119.835	119.984
A8	A(2,3,8)	119.606	119.529
A9	A(4,3,8)	120.559	120.487
A10	A(3,4,5)	120.348	120.226

A11	A(3,4,9)	120.168	120.267
A12	A(5,4,9)	119.484	119.507
A13	A(4,5,6)	120.049	120.027
A14	A(4,5,10)	121.495	121.331
A15	A(6,5,10)	118.456	118.643
A16	A(1,6,5)	119.463	119.616
A17	A(1,6,11)	120.342	120.235
A18	A(5,6,11)	120.195	120.149
A19	A(6,11,14)	107.360	107.689
A20	A(1,12,13)	109.550	110.095
D1	D(6,1,2,3)	0.000	-0.001
D2	D(6,1,2,7)	-180.000	-180.000
D3	D(12,1,2,3)	180.001	179.996
D4	D(12,1,2,7)	0.001	-0.003
D5	D(2,1,6,5)	0.001	0.001
D6	D(2,1,6,11)	180.001	-179.999
D7	D(12,1,6,5)	-180.000	-179.996
D8	D(12,1,6,11)	0.000	0.004
D9	D(2,1,12,13)	0.040	0.036
D10	D(6,1,12,13)	-179.959	-179.967
D11	D(1,2,3,4)	-0.001	0.000
D12	D(1,2,3,8)	-180.001	-180.000
D13	D(7,2,3,4)	180.000	179.999
D14	D(7,2,3,8)	0.000	-0.001
D15	D(2,3,4,5)	0.001	0.001
D16	D(2,3,4,9)	-180.000	-180.000
D17	D(8,3,4,5)	-179.999	-180.000
D18	D(8,3,4,9)	0.000	0.000
D19	D(3,4,5,6)	0.000	-0.001
D20	D(3,4,5,10)	179.999	179.999
D21	D(9,4,5,6)	-179.999	-180.000
D22	D(9,4,5,10)	-0.001	-0.001
D23	D(4,5,6,1)	-0.001	-0.001
D24	D(4,5,6,11)	-180.001	180.000
D25	D(10,5,6,1)	-179.999	-180.000
D26	D(10,5,6,11)	0.001	0.001
D27	D(1,6,11,14)	0.016	0.014
D28	D(5,6,11,14)	-179.984	-179.986

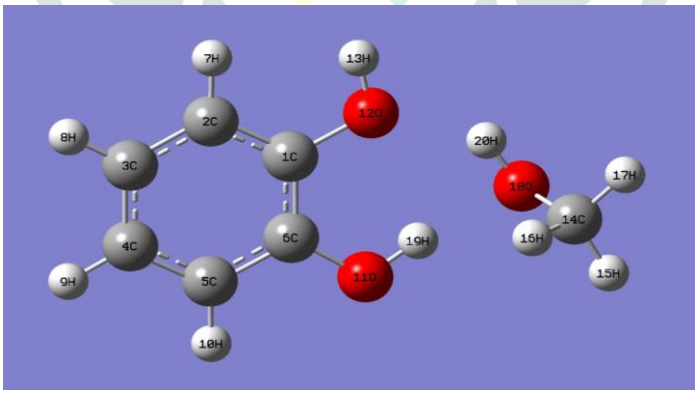


Fig.2. Optimized structure of Catechol+Methanol

Table-3. Mulliken atomic charges of Catechol+Methanol system

Atom no.	Atom	Charges
1	C	0.251199
2	C	-0.180848
3	C	-0.137619
4	C	-0.130801
5	C	-0.174699
6	C	0.328244
7	H	0.129402
8	H	0.128443
9	H	0.134055
10	H	0.14924
11	O	-0.666117
12	O	-0.446052
13	H	0.288317
14	C	-0.267372
15	H	0.136744
16	H	0.096409
17	H	0.129922
18	O	-0.645784
19	H	0.43866
20	H	0.438658

Table-4. Optimized Parameters of catechol+Methanol system

Optimized Parameters (Distance in Angstroms and Angle in Degrees)		
Number	Atoms	Å / degree
R1	R(1,2)	1.3943
R2	R(1,6)	1.4108
R3	R(1,12)	1.3828
R4	R(2,3)	1.3973
R5	R(2,7)	1.0882
R6	R(3,4)	1.3951
R7	R(3,8)	1.0858
R8	R(4,5)	1.3958
R9	R(4,9)	1.0863
R10	R(5,6)	1.3994
R11	R(5,10)	1.0863
R12	R(6,11)	1.3598
R13	R(11,19)	0.9902
R14	R(12,13)	0.9709
R15	R(12,20)	1.9438
R16	R(14,15)	1.0923
R17	R(14,16)	1.0971
R18	R(14,17)	1.0967
R19	R(14,18)	1.4324
R20	R(18,19)	1.7569
R21	R(18,20)	0.9758
A1	A(2,1,6)	120.351
A2	A(2,1,12)	121.947
A3	A(6,1,12)	117.7
A4	A(1,2,3)	120.614
A5	A(1,2,7)	119.038
A6	A(3,2,7)	120.348
A7	A(2,3,4)	119.483
A8	A(2,3,8)	119.698
A9	A(4,3,8)	120.82

A10	A(3,4,5)	119.941
A11	A(3,4,9)	120.424
A12	A(5,4,9)	119.634
A13	A(4,5,6)	121.283
A14	A(4,5,10)	121.072
A15	A(6,5,10)	117.645
A16	A(1,6,5)	118.325
A17	A(1,6,11)	123.775
A18	A(5,6,11)	117.889
A19	A(6,11,19)	113.091
A20	A(1,12,13)	109.288
A21	A(1,12,20)	129.204
A22	A(13,12,20)	117.596
A23	A(15,14,16)	108.942
A24	A(15,14,17)	108.815
A25	A(15,14,18)	107.087
A26	A(16,14,17)	109.112
A27	A(16,14,18)	111.706
A28	A(17,14,18)	111.101
A29	A(14,18,19)	109.881
A30	A(14,18,20)	107.53
A31	A(19,18,20)	86.6764
A32	A(11,19,18)	175.424
A33	A(12,20,18)	138.377
D1	D(6,1,2,3)	0.6337
D2	D(6,1,2,7)	-179.82
D3	D(12,1,2,3)	-178.9
D4	D(12,1,2,7)	0.6451
D5	D(2,1,6,5)	-0.7039
D6	D(2,1,6,11)	-179.46
D7	D(12,1,6,5)	178.852
D8	D(12,1,6,11)	0.0979
D9	D(2,1,12,13)	-0.4766
D10	D(2,1,12,20)	-157.23
D11	D(6,1,12,13)	179.975
D12	D(6,1,12,20)	23.2207
D13	D(1,2,3,4)	-0.1256
D14	D(1,2,3,8)	179.824
D15	D(7,2,3,4)	-179.67
D16	D(7,2,3,8)	0.2817
D17	D(2,3,4,5)	-0.2964
D18	D(2,3,4,9)	179.941
D19	D(8,3,4,5)	179.755
D20	D(8,3,4,9)	-0.0076
D21	D(3,4,5,6)	0.2142
D22	D(3,4,5,10)	-179.67
D23	D(9,4,5,6)	179.979
D24	D(9,4,5,10)	0.0915
D25	D(4,5,6,1)	0.284
D26	D(4,5,6,11)	179.112
D27	D(10,5,6,1)	-179.83
D28	D(10,5,6,11)	-0.9971
D29	D(1,6,11,19)	-13.617
D30	D(5,6,11,19)	167.624
D31	D(6,11,19,18)	-177.3
D32	D(1,12,20,18)	-37.6
D33	D(13,12,20,18)	167.256
D34	D(15,14,18,19)	81.6373
D35	D(15,14,18,20)	174.479

D36	D(16,14,18,19)	-37.564
D37	D(16,14,18,20)	55.2779
D38	D(17,14,18,19)	-159.66
D39	D(17,14,18,20)	-66.819
D40	D(14,18,19,11)	-70.252
D41	D(20,18,19,11)	-177.7
D42	D(14,18,20,12)	-93.708
D43	D(19,18,20,12)	16.1004

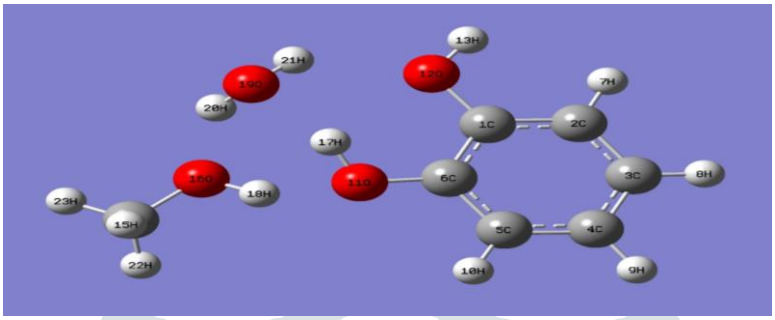


Fig.3. Optimized structure of Catechol+Methanol+Water

Table-5. Mulliken atomic charges of Catechol+Methanol+Water system

Atom no.	Atom	Charges
1	C	0.312824
2	C	-0.20156
3	C	-0.137891
4	C	-0.137382
5	C	-0.17097
6	C	0.324568
7	H	0.119431
8	H	0.128846
9	H	0.129029
10	H	0.138688
11	O	-0.712048
12	O	-0.680545
13	H	0.416086
14	C	-0.210686
15	H	0.14502
16	O	-0.649407
17	H	0.443611
18	H	0.425696
19	O	-0.818338
20	H	0.420904
21	H	0.412068
22	H	0.142316
23	H	0.159739

Table-6. Optimized Parameters of Catechol+Methanol+Water

Optimized Parameters (Distance in Angstroms and Angle in Degrees)		
Number	**Atoms**	**Å / degree**
R1	R(1,2)	1.3949
R2	R(1,6)	1.4087
R3	R(1,12)	1.3774
R4	R(2,3)	1.3974
R5	R(2,7)	1.0879
R6	R(3,4)	1.395
R7	R(3,8)	1.0858
R8	R(4,5)	1.3967
R9	R(4,9)	1.086
R10	R(5,6)	1.3962

R11	R(5,10)	1.0862
R12	R(6,11)	1.3697
R13	R(11,17)	0.9966
R14	R(11,18)	1.9873
R15	R(12,13)	0.971
R16	R(12,21)	2.1054
R17	R(14,15)	1.098
R18	R(14,16)	1.4297
R19	R(14,22)	1.0975
R20	R(14,23)	1.0926
R21	R(16,18)	0.9786
R22	R(16,20)	1.8624
R23	R(17,19)	1.7547
R24	R(19,20)	0.9861
R25	R(19,21)	0.9733
A1	A(2,1,6)	119.9784
A2	A(2,1,12)	122.566
A3	A(6,1,12)	117.4554
A4	A(1,2,3)	120.523
A5	A(1,2,7)	119.043
A6	A(3,2,7)	120.4332
A7	A(2,3,4)	119.7018
A8	A(2,3,8)	119.5986
A9	A(4,3,8)	120.6996
A10	A(3,4,5)	119.8689
A11	A(3,4,9)	120.465
A12	A(5,4,9)	119.6658
A13	A(4,5,6)	120.9064
A14	A(4,5,10)	121.1069
A15	A(6,5,10)	117.9865
A16	A(1,6,5)	119.0185
A17	A(1,6,11)	122.8239
A18	A(5,6,11)	118.1504
A19	A(6,11,17)	112.913
A20	A(6,11,18)	119.7656
A21	A(17,11,18)	84.7982
A22	A(1,12,13)	109.2614
A23	A(1,12,21)	131.4827
A24	A(13,12,21)	118.4822
A25	A(15,14,16)	112.0356
A26	A(15,14,22)	108.8685
A27	A(15,14,23)	108.7033
A28	A(16,14,22)	111.3484
A29	A(16,14,23)	107.1346
A30	A(22,14,23)	108.6537
A31	A(14,16,18)	107.8882
A32	A(14,16,20)	115.0124
A33	A(18,16,20)	88.728
A34	A(11,17,19)	157.117
A35	A(11,18,16)	147.5663
A36	A(17,19,20)	89.6254
A37	A(17,19,21)	89.1576
A38	A(20,19,21)	104.3155
A39	A(16,20,19)	151.8923
A40	A(12,21,19)	131.2059
D1	D(6,1,2,3)	0.541
D2	D(6,1,2,7)	-179.7905
D3	D(12,1,2,3)	-179.6379
D4	D(12,1,2,7)	0.0306
D5	D(2,1,6,5)	-0.6243
D6	D(2,1,6,11)	-179.625
D7	D(12,1,6,5)	179.5456
D8	D(12,1,6,11)	0.5449
D9	D(2,1,12,13)	-1.9433
D10	D(2,1,12,21)	167.5644

D11	D(6,1,12,13)	177.8821
D12	D(6,1,12,21)	-12.6102
D13	D(1,2,3,4)	-0.1148
D14	D(1,2,3,8)	179.8788
D15	D(7,2,3,4)	-179.7787
D16	D(7,2,3,8)	0.2149
D17	D(2,3,4,5)	-0.2212
D18	D(2,3,4,9)	179.9495
D19	D(8,3,4,5)	179.7852
D20	D(8,3,4,9)	-0.0441
D21	D(3,4,5,6)	0.1304
D22	D(3,4,5,10)	-179.7141
D23	D(9,4,5,6)	179.9611
D24	D(9,4,5,10)	0.1166
D25	D(4,5,6,1)	0.2916
D26	D(4,5,6,11)	179.3393
D27	D(10,5,6,1)	-179.8591
D28	D(10,5,6,11)	-0.8115
D29	D(1,6,11,17)	-10.2556
D30	D(1,6,11,18)	87.1184
D31	D(5,6,11,17)	170.7354
D32	D(5,6,11,18)	-91.8906
D33	D(6,11,17,19)	126.0336
D34	D(18,11,17,19)	5.853
D35	D(6,11,18,16)	-117.0213
D36	D(17,11,18,16)	-3.5495
D37	D(1,12,21,19)	30.6347
D38	D(13,12,21,19)	-160.644
D39	D(15,14,16,18)	58.456
D40	D(15,14,16,20)	-38.7163
D41	D(22,14,16,18)	-63.7379
D42	D(22,14,16,20)	-160.9101
D43	D(23,14,16,18)	177.5857
D44	D(23,14,16,20)	80.4135
D45	D(14,16,18,11)	-113.1211
D46	D(20,16,18,11)	2.8065
D47	D(14,16,20,19)	103.5764
D48	D(18,16,20,19)	-5.6119
D49	D(11,17,19,20)	-7.2572
D50	D(11,17,19,21)	-111.5803
D51	D(17,19,20,16)	5.4612
D52	D(21,19,20,16)	94.4962
D53	D(17,19,21,12)	-11.1286
D54	D(20,19,21,12)	-100.527

First, the structures of the solvent were optimized and stable conformations are obtained. The optimized structure of alcohols then combined with water and catechol molecule as shown in Fig. 4 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 are given in Table-7. From this Table, polarizability of single molecule is observed to be increases when it's combination with other molecule. Similarly, dipole moments are also increase with polarizability. Table-7 denoted with abbreviations for molecular systems as:-W: Water, M: Methanol, C: Catechol.

Table 7- Experimental and Calculated υ-OH (–OH str.freq.) along with dipole moment isotropic polarizability (α), -OH bond distance, Intermolecular H-bond distance for pure substance, binary solvents and ternary solution by DFT/ B3LYP method at 6-31G(d) basis set

System	Phase/ Media	Dipole Moment (Debye)	(α) Bohr^3	Exp. υ-OH cm^{-1}	Alcoholic/ Phenolic υ-OH cm^{-1}	Alcoholic(-OH) Bond Dist. (^{0}A)	Intermolecular H-Bond Dist.(^{0}A)
C	Gas	2.518	63.59	3441, 3321.4	3627.4, 3574.2	-	-
	Water	3.275	82.92		3606.96,3557.3	-	-
W	Gas	2.095	5.22	-	3584.2(sy.str.) 3701.3(Uns.str.)	-	-
	Water	2.314	5.52		3584.8(sy.str.) 3684.6(Uns.str.)	-	-
M	Gas	1.694	15.70	3347	3609.22	0.9687	-
	Water	1.974	17.99		3606.66	0.9696	-
	Water	1.845	44.69		3602.54	0.9699	-
	Water	3.464	25.17		3477.48	0.9821	1.8328
	Water	5.058	91.71		3603.35, 3219.87	-	1.9397 1.7571
MC	Gas	3.515	82.46	3360	3537.34	0.9748	1.9166
	Water	4.895	104.84		3522.66	0.9758	1.9474
	Water	5.018	131.85		3520.84	0.9761	1.9590
WMC	Gas	2.108	90.15	3375.43	3456.05	0.9790	1.9537
	Water	2.654	113.13		3463.45	0.9786	1.9873
	Water	5.268	139.65		3486	0.9773	2.0655

[Abbreviations:-W: Water, M: Methanol, C: Catechol]

HOMO-LUMO structures are shown in Fig. 5 with its energy gap. HOMO-LUMO energy gap given in Table-8 gives an idea about the stability/ reactivity of the species. More the energy gap, stable is the system. As energy gap decreases reactivity is increases. Different forms of energy of these molecular systems are given in Table-9.

Table 8-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)
C	Gas	-5.624	0.219	5.843
	Water	-8.179	-4.047	4.132
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
	Water	-6.794	1.588	8.382
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
	Water	-5.688	0.113	5.801
WMC	Gas	-5.783	0.100	5.883
	Water	-5.826	0.046	5.872
	Water	-5.806	0.048	5.855

Table 9- Theoretical Thermodynamic functions calculated by DFT/B3LYP method at 6-31G (d) basis set

System	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
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
	Water	-270.77954	83.28833	184.2053	88.996	28.379	94.04
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
	Water	-577.05621	137.9132	689.0442	146.41	48.806	122.72
WMC	Gas	-574.84195	118.5118	622.6267	126.99	47.508	118.91
	Water	-574.85337	118.0573	622.1720	126.60	47.891	118.91
	Water	-653.48688	153.9886	840.0846	163.97	57.707	129.19

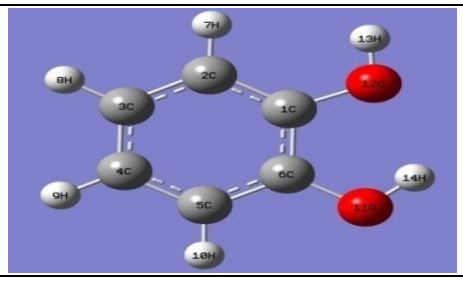
Chemical reactivity:

HOMO-LUMO energy gap used to calculate global chemical reactivity indices for different molecular system by using Eq. (1-7). These equation are also used to calculate chemical hardness (Ƞ), chemical softness (ϭ), electronegativity (χ), electrochemical potential (μ), global electrophilicity index (ω), electron affinity (A), ionization energy (I) which are given in Table 10. From this Table, it is observed that chemical hardness (Ƞ) and ionization energy (I) are highest for pure Catechol than solvent: W, M. Further decrease is observed when these catechol combined with solvent: WC, MC and WMC. This trend of chemical hardness (Ƞ) indicates the stability of the system and hence required more energy for ionization.

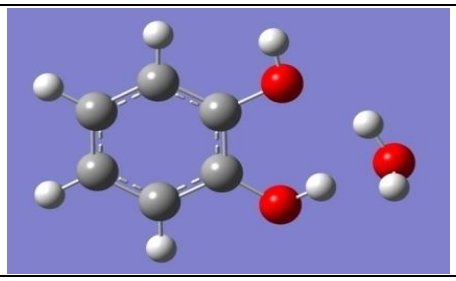
Table 10- Global chemical reactivity indices.
[Chemical Hardness (Ƞ), Chemical Softness (ϭ), Electronegativity (χ), Electrochemical potential (μ), Global electrophilicity index (ω), Electron affinity (A), Ionization energy (I)]

System	Phase/ Media	Ƞ (eV)	ϭ (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
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
	Water	4.77	0.21	2.44	-2.44	0.62	-2.33	7.21
	Water	4.19	0.24	2.60	-2.60	0.81	-1.59	6.79
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
	Water	2.90	0.34	2.79	-2.79	1.34	-0.11	5.69
WMC	Gas	2.94	0.34	2.84	-2.84	1.37	-0.10	5.78
	Water	2.94	0.34	2.89	-2.89	1.42	-0.05	5.83
	Water	2.93	0.34	2.88	-2.88	1.42	-0.05	5.81

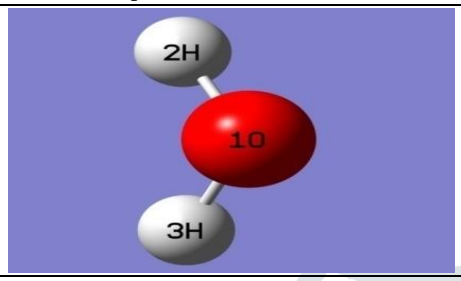
Fig. 4-Optimized structures of solute, solvents combinations by DFT method at B3LYP level using 6-31G(d) basis set.



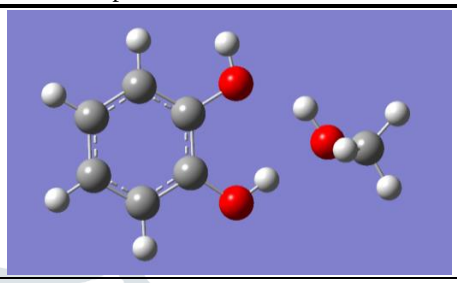
1-Optimized structure of **C**



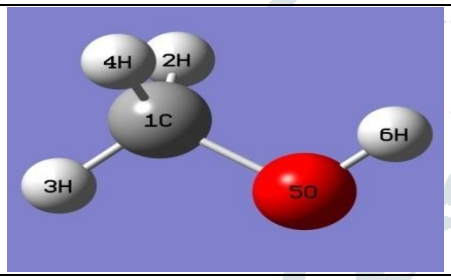
4-Optimized structure of **WC**



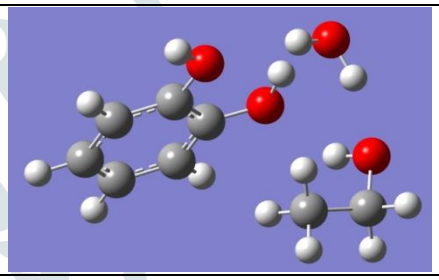
2-Optimized structure of **W**



5-Optimized structure of **MC**

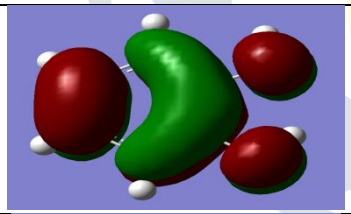
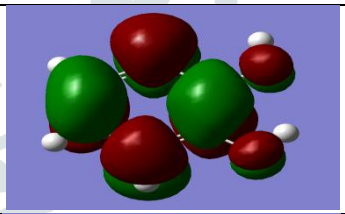
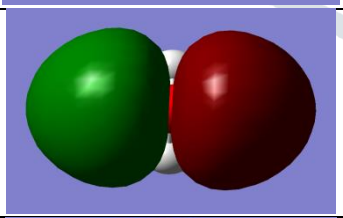
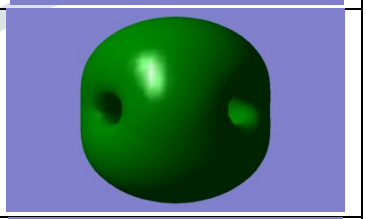
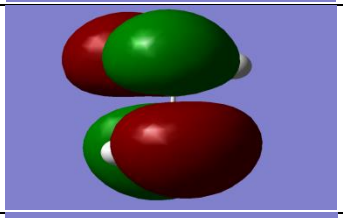
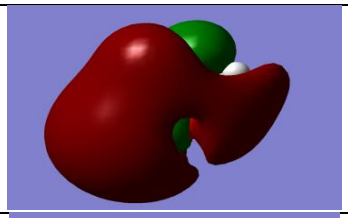
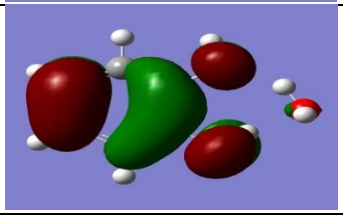
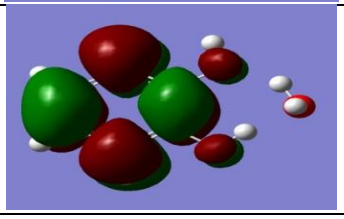


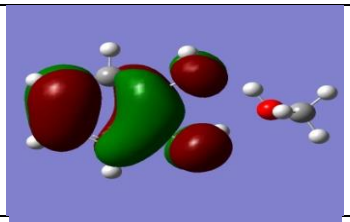
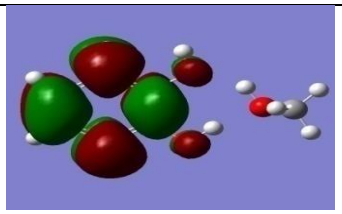
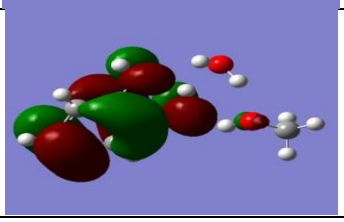
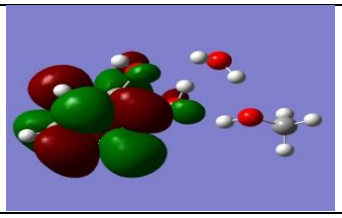
3-Optimized structure of **M**



6-Optimized structure of **WMC**

Fig. 5-HOMO, LUMO structures with LUMO-HOMO Energy Gap.

Molecule	HOMO	L-H E.G.(eV)	LUMO
C		Gas 5.843	
		Water 4.132	
W		Gas 9.628	
		Water 10.097	
M		Gas 9.246	
		Water 9.564	
WC		Gas 5.775	
		Water 5.809	

MC		Gas 5.787	
		Water 5.812	
WMC		Gas 5.883	
		Water 5.872	

IV. CONCLUSIONS:

Computational study of these molecules is found to be useful to get the optimized structures, stability, HOMO, LUMO, thermodynamic properties of pure catechol, water, methanol molecular system and their combinations to explain solute-solvent interaction. These data is useful in the field of solution chemistry and synthesis.

V. ACKNOWLEDGMENTS

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