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Prediction of Dielectric Constant (ϵ) for Phenol substituted, Using Quantitative Structure-Property Relationship (QSPR)

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Abstract

Quantitative structure–property relationship (QSPR) model is explored for the prediction of dielectric constant (ε) of phenol compounds. Six QSPR models for the expression of dielectric constant have been drawn up by employ the multiple regression approach. (Eqs 1-6) with the values of R^2 range from 0.717-0.9061, Ra^2 range from 0.7021-0.87253and the values of S range from 5.390-3.524166, while the values of F range from 45.786-27.046689. The results show excellent model by Eq 5 with high of R^2, Ra^2, F and minimum S by using five parameters [LogP, LUMO, HE, HOMO and D.M],was found and indicate that these parameters have important role in determining the value of dielectric constant.

Keywords: Phenol substituted; Predicted dielectric constant (ε); (QSPR) model.

1. Introduction

Quantitative structure–property/activity relationships (QSPR/QSAR) are effective branch from computational chemistry which depend on the molecular descriptors [1-4]. There are numerous applications for (QSPR/QSAR) including modelling of heat transition [5], rate constants of reaction [6], normal boiling points,[7-10] stability of complexes [11], mineral crystal lattice energy [12], solubility [13], biodegradation of organic compounds [14], water solubility of minerals [15] ,anti-cancer drug discovery [16] and anti-malarial activity [17].

Quantitative structure–property/activity relationships (QSPR/QSAR) are used in modelling of biological activity of 49 phenol derivatives against L1210 Leukaemia cells [18] . Dixit and Sikarwar were build QSAR modeling activity of phenol derivatives against Leukemia cells lines by used three descriptors Mor20e, Mor04m and RDF045m [19] while Yao et al was develop QSAR model for prediction of toxicities of 153 phenols by used support vector machines [20]. In the other hand Bosque and Sales introduced a Quantitative Structure−Property Relationship (QSPR) for the O−H bond dissociation energy (BDE) of a set of 78 phenols [21]. However , Xue et al used support vector machines to develop (QSPR) model of the O−H bond dissociation energy (BDE) of 78 substituted phenols [22]. Recently Achary made QSPR model for the prediction of dielectric constant of π conjugated organic compounds [23]. In this study we established quantitative structure – property relationships (QSPR) for predictive dielectric constant (ε) using descriptors calculated with density functional theory (DFT) to find factors that influence on dielectric constant of molecules understudy.

2. Modeling and Geometry Optimization

The quantum chemical calculations were performed for 20 compounds understudy with the Gaussian03 [24]. Geometrical optimizations were achieved applying Density Functional Theory (DFT) method at B3LYP/6-31G level of theory [25]. The experimental dielectric constant (**ε**) data of 20 phenol substituted compounds under study has been taken from reference [26]. Structures of 20 phenol substituted compounds shown in Figure.1 .

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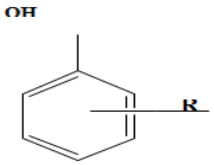
Fig-1. Molecular structure of compounds under study

No	R
1	Phenol
2	O- Chloro Phenol
3	M- Chloro Phenol
4	P- Chloro Phenol
5	O-Cresole
6	M-Cresole
7	P-Cresole
8	O-Cyclohexylphenol
9	P-Cyclohexylphenol
10	2,3-Dimethylphenol
11	2,4-Dimethylphenol
12	2,5-Dimethlphenol
13	3,4-Dimethylphenol
14	3,5-Dimethylphenol
15	O-Methoxyphenol
16	M-Methoxyphenol
17	P-Methoxyphenol
18	O-Nitrophenol
19	M-Nitrophenol
20	P-Nitrophenol



3. Results and Discussion

The multiple linear regressions (MLR) were performed between dielectric constant (**ε**) of compound and some quantum chemical descriptors to build QSPR models. Most important descriptors include in the QSPR models are the HOMO energy, LUMO energy, HOMO-LUMO energy gap (ΔE), Dipole moment, charge, Total Energy, Hydration Energy, refractivity, LogP, volume, surface (A), surface (G), can be directly related with experimental data of dielectric constant (**ε**). The 1 and 12 descriptor correlations of the dielectric constant (**ε**) were given in eqs (1-6) respectively and the resulting parametric models are visualized in figures. 2-6, along with statistical parameters of the regression.

The first model when form on from one parameter [LUMO] gave model with correlation coefficient R^2 values for this model of 0.717, as equation 1. The suggest that the dielectric constant (**ε**) increases with reduction values of this descriptor. Table 1. shows descriptors as the independent variables used for QSPR analysis of compounds.

Table-1. Descriptors as the independent variables used for QSPR analysis of compounds

No	LUMO	HOMO	D.M	T.E	Mass	pol	Ref	Log- p	H.E	Volum	Surf (G)	Surf (A)
1	-0.001	-0.223	1.5787	-307.388	94.11	11.07	27.75	1.76	-9.05	353.42	249.02	221.06
2	-0.015	-0.235	3.6835	-766.96	128.56	13	32.56	2.28	-7.62	400.78	275.83	249.25
3	-0.017	-0.239	3.7795	-766.963	128.56	13	32.56	2.28	-8.66	402.84	277.94	256.01
4	-0.019	-0.232	2.7522	-766.963	128.56	13	32.56	2.28	-8.81	402.92	277.1	257.02
5	0.005	-0.217	1.2772	-346.698	108.14	12.91	32.79	2.23	-6.61	407.89	276.5	251.16
6	-0.001	-0.22	1.2757	-346.697	108.14	12.91	32.79	2.23	-7.71	410.49	280.58	262
7	0.001	-0.214	1.6123	-346.696	108.14	12.91	32.79	2.23	-7.89	410.33	279.63	263.63
8	0.002	-0.219	1.5902	-542.009	176.26	21.31	53.94	3.64	-2.01	610.91	384.29	296.56
9	0.001	-0.214	1.6975	-542.01	176.26	21.31	57.99	2.14	-6.48	604.95	380.85	315.09
10	0.006	-0.215	0.9611	-386.004	122.17	14.74	37.83	2.7	-5.33	454.38	299.32	282.42
11	0.006	-0.21	1.2491	-386.005	122.17	14.74	37.83	2.7	-5.4	461.29	304.43	291.98
12	0.01	-0.212	1.5793	-386.006	122.17	14.74	37.83	2.7	-5.31	461.14	303.88	291.49
13	0.002	-0.211	1.3835	-386.002	122.17	14.74	37.83	2.7	-6.62	456.39	302.17	294.34
14	0.005	-0.215	1.6443	-386.005	122.17	14.74	37.83	2.7	-6.41	463.81	307.32	300.02
15	0.005	-0.203	2.285	-421.864	124.14	13.54	34.22	1.51	-8.29	430.88	291.85	257.61
16	0.007	-0.213	1.0108	-421.872	124.14	13.54	34.22	1.51	-10.6	434.42	294.72	274.31
17	-0.002	-0.202	3.0606	-421.869	124.14	13.54	34.22	1.51	-11.04	434.16	293.32	278.1
18	-0.097	-0.259	6.7351	-511.796	139.11	12.79	35.08	1.72	-11.28	418.74	286.85	256.9
19	-0.107	-0.256	6.4496	-511.807	139.11	12.79	35.08	1.72	-14.04	421.85	288.62	273.65
20	-0.101	-0.262	5.7241	-511.81	139.11	12.79	35.08	1.72	-14.34	422.04	289.81	275.38

3.1. Definition of Descriptors Used in This Study

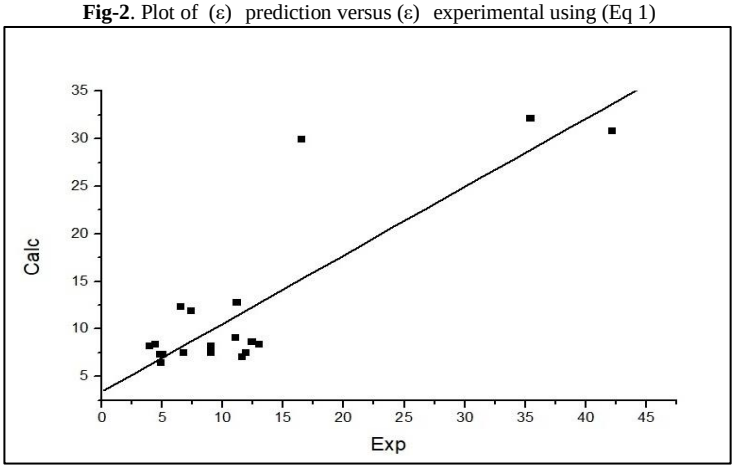
ΔE= Different between HOMO and LUMO is energy gaps in eV, LUMO= The energy of Lowest Unoccupied Molecular Orbital in eV, HOMO= The energy of Highest Occupied Molecular Orbital in eV, D.M= Dipole moment in debyes., H.E= Hydration Energy in Kcal/mol, Volume in Ang^3 , T.E= Total Energy in a.u., Surface (G): Surface area(Grid) , Surface (A): Surface area(Approx) . (ε) = dielectric constant

ε= -219.9487LUMO+8.60078 (Eq1)

R^2 = 0.717 F = 45.786 S = 5.390 Ra^2= 0.702

The relationship between the experimental data and predicted dielectric constant for phenol substituted illustrated in Figure 2**.**

Fig-2. Plot of (ε) prediction versus (ε) experimental using (Eq 1)

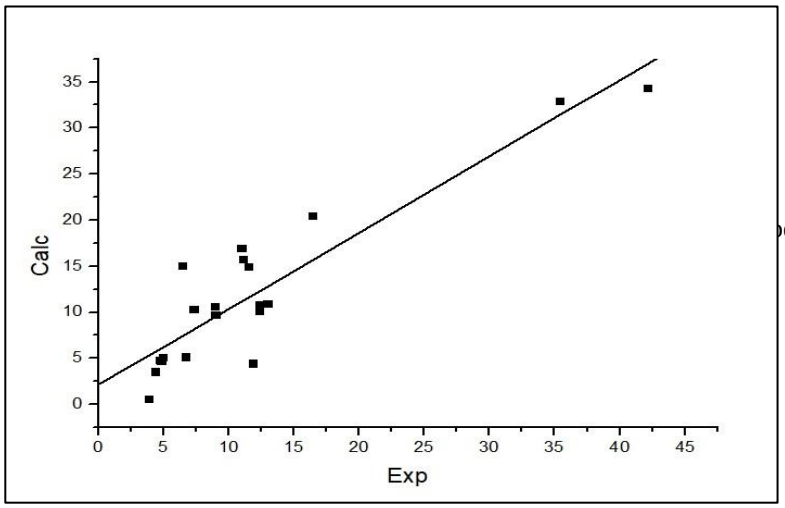


Second model of the dielectric constant (**ϵ**) of phenol compounds increases **ε** with increase Log p , in contrast **ε** values gain with lessening HE values. Figure 3. Shows the relationship between the experimental data and predicted dielectric constant.

ε = -50.6861+11.5714Logp+(-4.5341)HE.(Eq2).

R^2= 0.829 F =41.254 S = 4.315 Ra^2= 0.809

Fig-3. Plot of (ε) prediction versus (ε) experimental using (Eq 2)



perimental using (Eq 2).

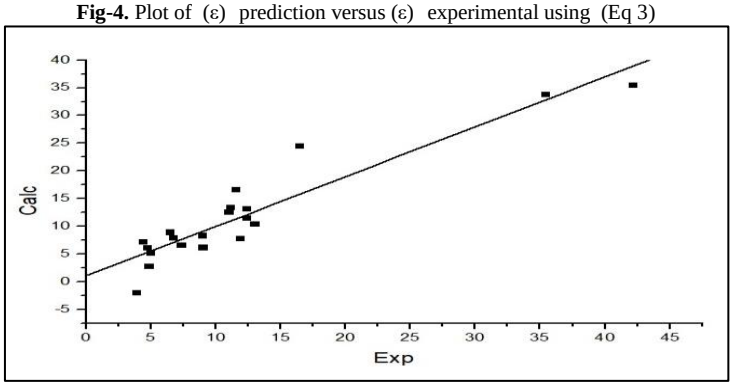
Three- parameter correlations of the phenols compounds were given in eq 3. In this equation it could be observe that increases of the correlation coefficient when depends on parameters [LUMO, T.E and H.E].

ε = -258.221LUMO+(-3.562)T.E+ (-2.0744)H.E (Eq3).

R^2 = 0.872 F = 58.378 S = 3.722 Ra^2= 0.857

The relationship between the experimental data and predicted dielectric constant (**ε**) illustrated in Figure 4

Fig-4. Plot of (ε) prediction versus (ε) experimental using (Eq 3)



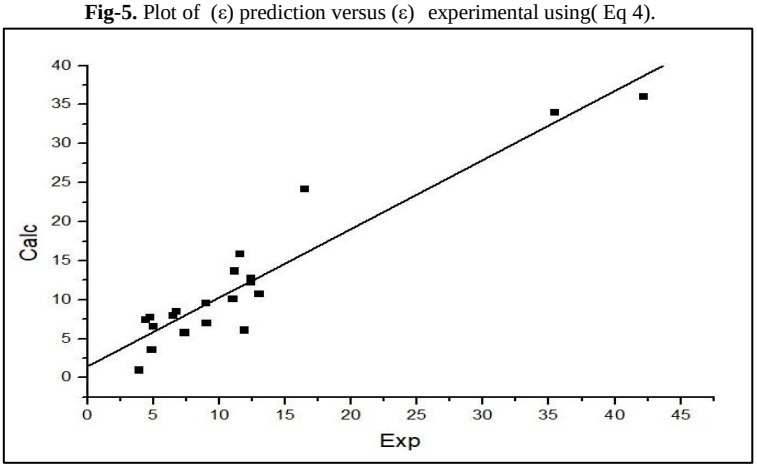
On other hand, when the adding of a parameters LogP to the equation 3. obtained on equation 4. with t h e

correlation coefficient 0.888. As seen from this resulting in a very slight enhancement of the correlation coefficient, in contrast standard error highest and a decrease of the *F*-test statistic, the relationship between the experimental data and predicted dielectric constant (**ε**) illustrated in Figure 5.

ε = 1.381LogP+(-318.365)LUMO+ (-4.6148)D.M+(-1.946)HE (Eq4).

R^2 = 0.888 F = 42.570 S = 3.591 Ra^2=0.867

Fig-5. Plot of (ε) prediction versus (ε) experimental using(Eq 4).

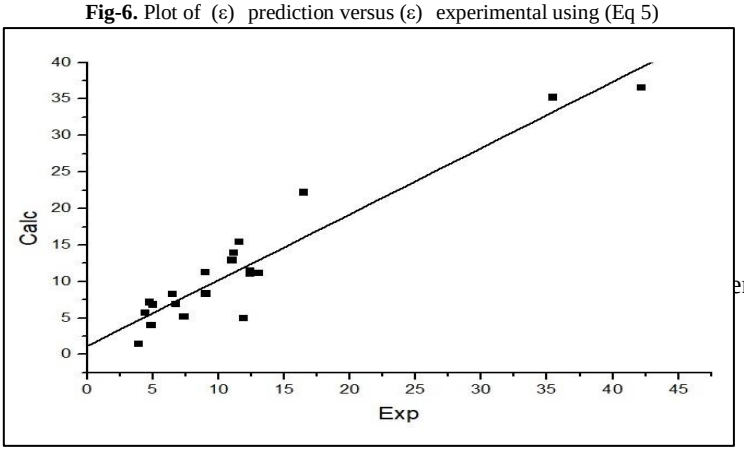


Excellent model equation when depends on five parameters [LogP, LUMO, HE, HOMO and D.M]. The resulting growth of the correlation coefficient, minimum standard error and a decrease of the *F*-test statistic, when adding of a parameter [HOMO] ,gave the good model predicted in this study Eq 5. This model equation depends on the five parameters[LogP, LUMO, HE, HOMO, D.M], have the significant rule suggesting the importance of the substituent's on the studied compounds on the predicted dielectric constant (**ε**) , the excellent relationship between the experimental data and predicted dielectric constant (**ε**) is shown in Figure 6.

ε = 6.920LogP+(-284.010)LUMO+ (-3.184)HE+(107.910)HOMO+ (-3.748) D.M (Eq5)

R^2= 0.9047 F = 35.619 S = 3.4306 Ra^2=0.87934

Fig-6. Plot of (ε) prediction versus (ε) experimental using (Eq 5)



erimental using (Eq 5).

While in the eq.6, six parameters, the good correlation coefficient R^2 obtained when add the descriptors T.E to E.q5, obtained on equation Eq6. Which has six parameters **[**T.E, LogP, LUMO, HE, HOMO and D.M]. As seen from this resulting in a very minor improvement of the correlation coefficient, The excellent relationship between the experimental and estimated dielectric constant (**ε**) is shown in Figure 7**.**

ε = 3.43077388296063E-03T.E+(-3.2969)D.M+ (-3.1352921)HE+(6.963)LogP+ (-268.7705) LUMO + (103.389) HOMO (Eq 6)

R^2= 0.906 F = 27.046 S = 3.524 Ra^2= 0.872

Fig-7. Plot of (ε) prediction versus (ε) experimental using (Eq 6)

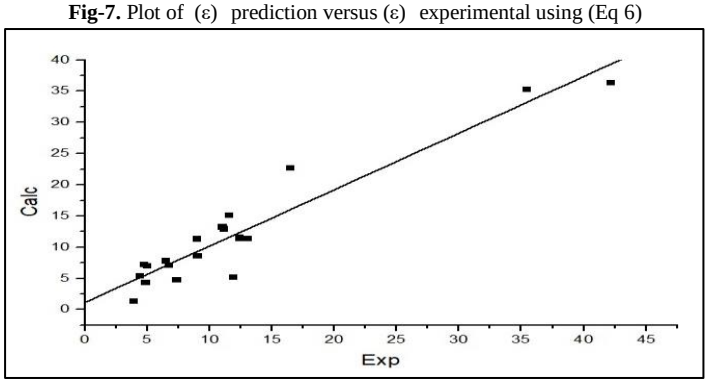


Table-2. Statistical characters of the linear regressions models

No	Descriptors	R^2	F	S	Ra^2
1	LUMO	0.717	45.786	5.390	0.702
2	Logp -HE	0.829	41.254	4.315	0.809
3	LUMO+ T.E+H.E	0.872	58.378	3.722	0.857
4	LogP+ LUMO+ D.M+HE	0.888	42.570	3.591	0.867
5	LogP, LUMO, HE, HOMO, D.M	0.904	35.619	3.430	0.879
6	TE+D.M+HE+Logp+LUMO+HOMO	0.906	27.046	3.524	0.872

It is noticeable from the table 2. that the relations between descriptors which calculations in this study and experimental the dielectric constant **(ε)**values are excellent. It could be seen from Table 3 the calculated of the dielectric constant **(ε)** values obtain from Eq. 1-6 in this study and comparable with the experimental values.

Table-3. Estimated empirical data by Eq 1. & Eq 6.

No	(ε) (Exp)	Calc By Eq1	Calc By Eq2	Calc By Eq3	Calc By Eq4	Calc By Eq5	Calc By Eq6
	R^2	R^2=0.717	R^2=0.829	R^2=0.872	R^2=0.888	R^2=0.904	R^2=0.906
1	12.4	8.600	10.713	13.146	12.764	11.021	11.367
2	7.4	11.900	10.246	6.554	5.760	5.141	4.726
3	6.55	12.339	14.962	8.885	7.979	8.230	7.794
4	11.18	12.779	15.642	13.373	13.648	13.882	12.912
5	6.76	7.501	5.088	7.868	8.462	6.860	7.072
6	12.44	8.600	10.076	11.446	12.203	11.465	11.61
7	13.05	8.380	10.892	10.362	10.681	11.140	11.366
8	3.97	8.160	0.547	-2.013	0.966	1.430	1.365
9	4.42	8.380	3.457	7.134	7.419	5.707	5.367
10	4.81	7.281	4.723	6.081	7.760	7.152	7.177
11	5.06	7.281	5.041	5.2006	6.568	6.835	6.964
12	4.9	6.401	4.633	2.804	3.595	3.959	4.311
13	9.02	8.160	10.572	8.285	9.596	11.245	11.317
14	9.06	7.501	9.620	6.145	7.028	8.315	8.579
15	11.95	7.501	4.374	7.762	6.087	4.961	5.193
16	11.59	7.061	14.84	16.576	15.828	15.447	15.065
17	11.05	9.040	16.843	12.510	10.090	12.909	13.242
18	16.5	29.935	20.361	24.447	24.135	22.184	22.674
19	35.45	32.135	32.875	33.771	34.009	35.208	35.266
20	42.2	30.815	34.236	35.429	36.031	36.531	36.366

4. Conclusion

The values of R^2 for the QSPR models Eqs. 1-6 range from 0.717-0.9061, the values of Ra^2 range from 0.7021-0.87253, and the values of S in the Eqs. 1-6 range from 5.390-3.524, while the values of F range from 45.786-27.046689 which are statistically significant at the 99% level. The values of R^2, Ra^2 ,F and S suggest that the QSPR models Eqs. 1-6 are predictive and validate. From all the results the Eq 5. have smaller the value of S and the larger the value of F, the better the QSPR model.

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