STUDYING OF CORRELATION BETWEEN THE MOLECULAR STRUCTURE AND THE CORROSION INHIBITING EFFECT OF SOME PYRIMIDNE COMPOUNDS

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Abstract

Quantum chemical calculations were performed on the pyrimidne and it is derivatives that it use as corrosion inhibitors of iron electrode, using the semi–empirical method AM1. The highest occupied molecular orbital energy, lowest unoccupied molecular orbital energy, dipole moment and the total of electronic energies of the molecules is calculated. the assessment of quantum chemical and corrosion inhibition efficiency studies were carried out to investigate whether any clear links exist between the results of quantum chemical calculations and inhibition efficiencies experimental of pyrimidine and it is derivatives by using a linear model encompassing the charge transfer resistance " R_t ". Regression equations, with more reliable of correlation coefficients were derived between R_t and the molecular calculations. The significant correlations is evident indicated that the variation of the corrosion inhibition with the structure of the inhibitors may be explained in terms of electronic properties.

Keywords: Corrosion, corrosion inhibition, quantum chemical calculations, charge transfer resistance, semi–empirical method.

Introduction

The main strategy to prevent electrochemical corrosion is the metal isolation from corrosive agents in the most effective possible manner (1). Among the different methods available, the use of inhibitors is one of the most practical methods for corrosion protection (2-6). Aqueous solution of acids are among the most corrosive media. The rate at which metals are destroyed in acidic media is very high, especially when soluble corrosion products are formed (7). Although, in recent years some techniques such as in-situ interfacial investigations have been applied to the experimental studies of corrosion inhibitors (8). The study of material corrosion processes and their inhibition by organic inhibitors is a very active field of research (9). Computational chemistry is the quantitative modeling of chemical phenomena by computer – implemented techniques (10). Chemical calculations that can predict the outcome of molecular interactions and allow us to understand chemical reactivity are important tools in chemical research. The behavior of atoms and molecules is characterized by some parameters that chemists have extracted from their experience and used for predication of chemical reactivity (11). The electronic structure of the organic inhibitors is the most effective characteristic on the corrosion inhibition efficiency. For proper selection of inhibitors, electrochemical techniques coupled with surface analytical techniques can be used but a need exists for a systematic approach for characterization of the interaction between the organic inhibitor molecule and the metal. It is very important to clarify the interactions between inhibitor molecules and the metal surface in order to search new and efficient corrosion inhibitors (12). Theoretical approaches provide means of analyzing these interactions and there are many reports related with this area (13-20). Recently, it was reported that pyrimidine and it is derivatives had been used as corrosion inhibitors of the iron electrode (21). There are few papers dealing with the quantum chemical study of the corrosion inhibition of iron. The task of this paper is to study the inhibition mechanism and proposed the linear resistance model by means of a quantum chemical method, based on the electrochemical experiments.

Methods of Calculations

All the calculations were carried out using Restricted Hartree–Fock (RHF) level using AM1 " Austin Model 1" semi-empirical SCF-MO method in the computer program package (HyperChem. Professional Release 8.0.3 for windows molecular modeling system, from Hypercube Inc. USA). The calculation were implemented on an Compaq Presario V6430EE Notebook PC, Microprocessor 1.86 GHz Intel® Pentium® dual core processor T2130 ; (Microprocessor Cache, 1 MB Level 2 cache) with memory 1024 MB. Molecular structure were optimized to a gradient norm of < 0.01 in the vacuo phase. As an optimization procedure, the built-in Polack-Ribiere algorithm was used. In previous work that it completed by H.S.Awad and S. Abedl Gawad (22) the percent inhibition efficiency, P%, is calculated by polarization resistance obtained from Nyquist plots according to the equation :

$$P\% = [R_p - R_{p\,(inh.)} / R_p\,] \times 100 \ldots\ldots\ldots\ldots\ (1),$$

where $R_{p(inh.)}$; R_p are the polarization resistance values with and without inhibitor, respectively. Equation one is a starting point for this model. The P% according to equation one is calculated by the charge transfer resistance, the $R_{p\ (inh.)}$ evident to find the inhibition efficiency. Thus, the charge transfer resistance can be correlated with the calculated quantum chemical parameters in my proposed QSAR model. For this purpose, the LR model have been developed by four parameters include, the dipole moment, the energy of the highest occupied molecular orbital, the lowest unoccupied molecular orbital and the electronic energy of molecular. The concentration may be considered in LR model. The general equation of QSAR linear model can be expressed as follows :

$$R_{ti} = \sum_i (A\mu + BE_{HOMO} + CE_{LUMO} + DE_{electronic\ energy}) \times C_{inh.} \ldots\ldots\ldots\ldots\ (2).$$

Where i refers to the number of the experiment, R_{ti} the charge transfer resistance ; A, B, C, D are the regression coefficient of the calculated quantum chemical parameters for the molecular and $C_{inh.}$ denotes the concentration of the inhibitor.

Results and Discussion

In order to investigate the effect of subsistent on the inhibition mechanism and efficiency, quantum chemical calculations were preformed. Geometric structures and electronic of pyrimidne and series of it is derivatives used as corrosion inhibitors were calculated with AM1 semi-empirical method. The studied molecules in this work and experimentally observed the charge transfer resistance R_t and percent inhibitors efficiencies(22) are given Table (1, 2), respectively.

Quantum chemical parameters such as the energy of the highest occupied molecular orbital, E_{HOMO}; the energy of lowest unoccupied molecular orbital, E_{LUMO} dipole moment (μ); electronic energy are calculated and summarized in Table (1, 2). The studied molecules in Table (1, 2) were divided into two groups according to their behaviors to make systematic studies between structures and the charge transfer resistance(R_t). The first group includes set one : pyrimidine, 2-methyl pyrimidine, 2-hydroxy pyrimidine hydrochloride, 2- mercapto pyrimidine and the second group includes set two : 2,4-diaminopyrimidine, triaminopyrimidine, 2,4 diamino -6-hydroxpyrimidine, 2,4-diamino-6-mercapto pyrimidine, in other words, the first group includes the mono substituted groups. Experimental and calculated values of the charge transfer resistance (R_t) are reported in Tables (1-4) and Figs.(1–4) for the pyrimidine and it is derivatives. The regression equation for the first group (Table (1)) obtained by linear resistance model (LR) that it proposed by Bentiss(15) for the study of interaction of corrosion organic inhibitors with metal surface was :

$$R_t=135.575+(-3821.165\mu-2636.257HOMO\text{-}40410.9LUMO) \times C_{inh.} \ldots\ldots\ldots\ (3)$$

N=20 R square = 0.665 Adjusted R square=0.603 F = 10.604. And, the regression equation for the second group (Table (2)) by linear resistance model (LR) was :

$$R_t=196.582+(-33676.2\mu-95174.5HOMO\text{-}154LUMO) \times C_{inh.} \ldots\ldots\ldots\ (4)$$

N=20 R square = 0.866 Adjusted R square = 0.841 F=34.513 . Where R square denotes the correlation coefficient, N is the total number of experimental impedance and F denotes the ratio of two mean squares "the sum of square regression divided by the number of degree of freedom is the mean square for regression ", R adjusted R square, denotes the percent of the variance can be predicate from independent variable $^{(22-23)}$.

The best regression equation for the first group (Table (3)) by using the modified model of linear resistance in this work was :

$$R_t = 134.134 + (-11944.8\mu + 1035.123\,\text{HOMO} - 7297\,\text{LUMO} - 0.448E_{\text{Electronnic energy}}) \times C_{\text{inh.}} \quad \ldots\ldots(5);$$

N=20, R square = 0.738, R adjusted R square = 0.668, F = 10.546. And the best regression equation for the second group (Table (4)) by modified of resistance in this work was:

$$R_t=194.784+(923273.5\mu+332843.1\,\text{HOMO}-942130\,\text{LUMO}-13.601E_{\text{Electronic energy}}) \times C_{\text{inh.}} \quad \ldots\ldots(6),$$

N = 20, R square = 0.967, R adjusted R square = 0.958, F = 108.879.

Use the modified model of linear resistance that it is dependent on the calculate the electronic energy$^{(23)}$ of molecule have been elaborated the linear resistance model (LR) that it proposed by Bentiss$^{(15)}$. The values of R square, R adjusted square and F can be more reliable and asserted as true with a 95% level of confidence $^{(23,24)}$ " the model is significance " in regression equation 5, 6. As shown in Figs. (3, 4) if it compared with Figs. (1, 2) that include drawing the relationship between the experimental charge transfer resistance and the calculated charge transfer resistance, the correlation between derivatives was better (R square = 0.7377, R square = 0.9667), respectively. A highly significant correlation coefficients was obtained for the second group have been predicted the high protection efficiency values for this molecules. The established QSAR equation equations (5, 6) shows the sign of HOMO and LUMO coefficient which respectively positive for HOMO and negative for LUMO, indicate the importance of the band gap energy. This means, the corrosion inhibition seems to be supported by the band gap energy effectively. The values of the calculation coefficient respectively for the HOMO and LUMO energies are comparable to those calculated for the mono substituted pyrimidine. However, if we compared the corrosion inhibition efficiency between two groups of molecules the difference may be explained by a weaker influence of dipole moment μ. Moreover, the percent inhibition efficiencies increase in the second group when the molecules have less negative HOMO energies because of the E_{HOMO} often is associated with the electron donating ability of the molecule. This fact proves that d-orbital of metal accepted electrons from the pyrimidine compounds and feedback from between the metal and inhibitor molecules. Forming of feedback bond increases chemical adsorption of pyrimidine molecules on the metal surface and so increase the inhibition efficiencies of these compounds. More generally, the high inhibition efficiency of the molecule can be also be explained by the localized and the distribution of the HOMO and LUMO densities along the molecules. Effectively, Fig.(5) clearly shows that for the second group of pyrimidine compounds, the HOMO and LUMO densities is support by the more the nitrogen atoms " amino group " with oxygen and sulphur atoms in the inhibitor molecules, compounds 5, 6, 7 and 8, respectively. The highest values of the HOMO density were found in the vicinity of the sulphur, clearly indicating the nucleophilic center is sulphur atom " compound 8 ". Thus, the bond with the metal from sulphur will be easily formed rather than nitrogen and oxygen atoms. This indicates that the mercapto–containing compound exhibited the best inhibition, followed by that containing the amino group and then that with the hydroxyl group attached to the pyrimidine ring. This concurrent with the inhibition efficiency that it presented in Table (2), follows the order$^{(21)}$, com.8> com. 7 > com6 > com5.

The significant correlation indicated that the variation of the corrosion inhibition with the structure of the inhibitors may be explained in terms of electronic properties. In present work, the corrosion inhibition efficiency can be explained not only in terms of electron orbital analysis but also seems to depend on the geometry of these molecules. The difference in their inhibitive action can be explained on the basis of the number amino group and substituted by the hydroxyl or mercapto groups instead of the amino group in pyrimidine ring which contribute to the chemisorption strength through the donor – acceptor bond between the non–bonding electron pair and the vacant orbital of the metal surface. Thus, the results so far indicated that introducing a single substituent group into the pyrimidine ring improved it is inhibition effect to a different extent depending on the characteristics of the substituent group and by increasing the number of these groups would continue to increase the effectiveness of pyrimidine inhibitors.

Conclusion

It can be concluded that some of the key quantum chemical parameters computed using AM1 method may will be able to explain the inhibition mechanism of corrosion of iron in acidic solution. These are mainly dipole moment, the energies of the highest occupied, lowest unoccupied and electronic energy. The variation of the corrosion inhibition with the structure of the inhibitors may be explained in terms of electronic properties, this prove that the relationships of correlation is significant. The percent efficiency protection of corrosion for pyrimidine inhibitors may be explain in terms of molecular parameters. Using QSAR approach may establish a direct correlation for the first and second groups of molecules that it studied, between the molecular structure and efficiency protection by using a LR model joining the charge transfer resistance to chemical quantum parameters. Using the model that it include on the electronic energy have been given the statistics parameters is more reliable.

Table (1)

Shows the experimental and calculated the R_t values and the quantum chemical parameters of the first group of pyrimidine inhibitors used to derive regression equation three.

Com.	**Inhibitor Name**	**Concentration "M"**	**Protection efficiency**	**R_t Ωcm^2 Exp.**	**μ Debye**	**E_{HOMO} eV**	**E_{LUMO} eV**	**$E_{ele.energy}$ Kcal/mol**	**R_t Ωcm^2 Calcu.**
1	pyrimidine	1×10^{-6}	33.00	70	2.05	-10.58	-0.24	-79001.62	135.60
		1×10^{-5}	37.47	80	2.05	-10.58	-0.24	-79001.62	135.83
		1×10^{-4}	57.00	119	2.05	-10.58	-0.24	-79001.62	138.12
		1×10^{-3}	77.00	259	2.05	-10.58	-0.24	-79001.62	161.07
		1×10^{-2}	81.00	298	2.05	-10.58	-0.24	-79001.62	390.55
2	2-methylprimidine	1×10^{-6}	35.00	75	0.1	-9.04	0.24	-104852.02	135.78
		1×10^{-5}	40.00	83	0.1	-9.04	0.24	-104852.02	137.62
		1×10^{-4}	60.00	125	0.1	-9.04	0.24	-104852.02	156.01
		1×10^{-3}	80.00	263	0.1	-9.04	0.24	-104852.02	339.93
		1×10^{-2}	85.00	312	0.1	-9.04	0.24	-104852.02	2179.13
3	2-hydroxypyrimidine hydrochloride	1×10^{-6}	36.46	80	4.55	-10.28	-0.45	-137931.68	135.82
		1×10^{-5}	42.01	88	4.55	-10.28	-0.45	-137931.68	138.01
		1×10^{-4}	61.47	132	4.55	-10.28	-0.45	-137931.68	159.95
		1×10^{-3}	81.99	295	4.55	-10.28	-0.45	-137931.68	379.35
		1×10^{-2}	86.47	417	4.55	-10.28	-0.45	-137931.68	2573.36
4	2-mercaptopyrimidine	1×10^{-6}	38.47	82	2.28	-8.99	-0.44	-101211.66	135.80
		1×10^{-5}	44.00	91	2.28	-8.99	-0.44	-101211.66	137.79
		1×10^{-4}	63.00	139	2.28	-8.99	-0.44	-101211.66	157.73
		1×10^{-3}	84.00	334	2.28	-8.99	-0.44	-101211.66	357.13
		1×10^{-2}	88.53	527	2.28	-8.99	-0.44	-101211.66	2351.1

Table (2)

Shows the experimental and calculated the R_t values and the quantum chemical parameters of the second group of pyrimidine inhibitors used to derive regression equation four.

Com.	Inhibitor Name	Concentration "M"	Protection efficiency	R_t Ωcm^2 Exp.	μ Debye	E_{HOMO} eV	E_{LUMO} eV	$E_{ele.energy}$ Kcal/mol	R_t Ωcm^2 Calcu.
5	2,4-diaminopyrimidine	1×10^{-6}	41.00	86	1.79	-8.65	0.57	-132941.31	196.65
		1×10^{-5}	46.00	98	1.79	-8.65	0.57	-132941.31	197.29
		1×10^{-4}	64.99	152	1.79	-8.65	0.57	-132s941.31	203.68
		1×10^{-3}	86.99	417	1.79	-8.65	0.57	-132941.31	267.61
		1×10^{-2}	91.00	624	1.79	-8.65	0.57	-132941.31	906.86
6	2,4,6-triaminopyrimidine	1×10^{-6}	43.00	89	1.61	-8.42	0.89	-163279.73	196.61
		1×10^{-5}	48.00	100	1.61	-8.42	0.89	-163279.73	196.84
		1×10^{-4}	67.00	167	1.61	-8.42	0.89	-163279.73	199.17
		1×10^{-3}	90.00	500	1.61	-8.42	0.89	-163279.73	222.45
		1×10^{-2}	94.00	834	1.61	-8.42	0.89	-163279.73	455.24
7	2,4-diamino-6-hydroxypyrimidine	1×10^{-6}	45.00	93	1.43	-8.75	0.56	-165655.11	196.79
		1×10^{-5}	48.00	103	1.43	-8.75	0.56	-165655.11	198.63
		1×10^{-4}	67.00	179	1.43	-8.75	0.56	-165655.11	217.02
		1×10^{-3}	90.00	625	1.43	-8.75	0.56	-165655.11	400.98
		1×10^{-2}	94.00	1500	1.43	-8.75	0.56	-165655.11	2240.59
8	2,4-diamino-6-meracaptopyrimidine	1×10^{-6}	48.00	98	1.41	-8.57	0.32	-159478.75	196.84
		1×10^{-5}	53.00	108	1.41	-8.57	0.32	-159478.75	199.15
		1×10^{-4}	72.00	193	1.41	-8.57	0.32	-159478.75	222.27
		1×10^{-3}	95.00	834	1.41	-8.57	0.32	-159478.75	453.50
		1×10^{-2}	98.50	3333	1.41	-8.57	0.32	-159478.75	2765.80

Table (3)

Shows the experimental and calculated the R_t values and the quantum chemical parameters of the second group of pyrimidine inhibitors used to derive regression equation five.

Com.	Inhibitor Name	Concentration "M"	Protection efficiency	R_t Ωcm^2 Exp.	μ Debye	E_{HOMO} eV	E_{LUMO} eV	$E_{ele.energy}$ Kcal/mol	R_t Ωcm^2 Calcu.
1	pyrimidine	1×10^{-6}	33.00	70	2.05	-10.58	-0.24	-79001.62	134.15
		1×10^{-5}	37.47	80	2.05	-10.58	-0.24	-79001.62	134.31
		1×10^{-4}	57.00	119	2.05	-10.58	-0.24	-79001.62	135.88
		1×10^{-3}	77.00	259	2.05	-10.58	-0.24	-79001.62	151.60
		1×10^{-2}	81.00	298	2.05	-10.58	-0.24	-79001.62	308.81
2	2-methylprimidine	1×10^{-6}	35.00	75	0.1	-9.04	0.24	-104852.02	134.15
		1×10^{-5}	40.00	83	0.1	-9.04	0.24	-104852.02	134.32
		1×10^{-4}	60.00	125	0.1	-9.04	0.24	-104852.02	136.02
		1×10^{-3}	80.00	263	0.1	-9.04	0.24	-104852.02	153.04
		1×10^{-2}	85.00	312	0.1	-9.04	0.24	-104852.02	323.22
3	2-hydroxypyrimidine hydrochloride	1×10^{-6}	36.46	80	4.55	-10.28	-0.45	-137931.68	134.16
		1×10^{-5}	42.01	88	4.55	-10.28	-0.45	-137931.68	134.43
		1×10^{-4}	61.47	132	4.55	-10.28	-0.45	-137931.68	137.10
		1×10^{-3}	81.99	295	4.55	-10.28	-0.45	-137931.68	163.77
		1×10^{-2}	86.47	417	4.55	-10.28	-0.45	-137931.68	430.54
4	2-mercaptopyrimidine	1×10^{-6}	38.47	82	2.28	-8.99	-0.44	-101211.66	134.17
		1×10^{-5}	44.00	91	2.28	-8.99	-0.44	-101211.66	134.54
		1×10^{-4}	63.00	139	2.28	-8.99	-0.44	-101211.66	138.22
		1×10^{-3}	84.00	334	2.28	-8.99	-0.44	-101211.66	175.04
		1×10^{-2}	88.53	527	2.28	-8.99	-0.44	-101211.66	543.22

Table (4)

Shows the experimental and calculated the Rt values and the quantum chemical parameters of the second group of pyrimidine inhibitors used to derive regression equation six.

Com.	**Inhibitor Name**	**Concentration "M"**	**Protection efficiency**	**R_t Ωcm^2 Exp.**	**µ Debye**	**E_{HOMO} eV**	**E_{LUMO} eV**	**$E_{ele.energy}$ Kcal/mol**	**R_t Ωcm^2 Calcu.**
5	2,4-diaminopyrimidine	1×10^{-6}	41.00	86	1.79	-8.65	0.57	-132941.31	194.83
		1×10^{-5}	46.00	98	1.79	-8.65	0.57	-132941.31	195.23
		1×10^{-4}	64.99	152	1.79	-8.65	0.57	-132941.31	199.25
		1×10^{-3}	86.99	417	1.79	-8.65	0.57	-132941.31	239.47
		1×10^{-2}	91.00	624	1.79	-8.65	0.57	-132941.31	641.66
6	2,4,6-triaminopyrimidine	1×10^{-6}	43.00	89	1.61	-8.42	0.89	-163279.73	194.85
		1×10^{-5}	48.00	100	1.61	-8.42	0.89	-163279.73	195.45
		1×10^{-4}	67.00	167	1.61	-8.42	0.89	-163279.73	201.40
		1×10^{-3}	90.00	500	1.61	-8.42	0.89	-163279.73	260.99
		1×10^{-2}	94.00	834	1.61	-8.42	0.89	-163279.73	856.82
7	2,4-diamino-6-hydroxypyrimidine	1×10^{-6}	45.00	93	1.43	-8.75	0.56	-165655.11	194.92
		1×10^{-5}	48.00	103	1.43	-8.75	0.56	-165655.11	196.12
		1×10^{-4}	67.00	179	1.43	-8.75	0.56	-165655.11	208.12
		1×10^{-3}	90.00	625	1.43	-8.75	0.56	-165655.11	328.17
		1×10^{-2}	94.00	1500	1.43	-8.75	0.56	-165655.11	1528.65
8	2,4-diamino-6-meracaptopyrimidine	1×10^{-6}	48.00	98	1.41	-8.57	0.32	-159478.75	195.10
		1×10^{-5}	53.00	108	1.41	-8.57	0.32	-159478.75	197.95
		1×10^{-4}	72.00	193	1.41	-8.57	0.32	-159478.75	226.46
		1×10^{-3}	95.00	834	1.41	-8.57	0.32	-159478.75	511.56
		1×10^{-2}	98.50	3333	1.41	-8.57	0.32	-159478.75	3362.57

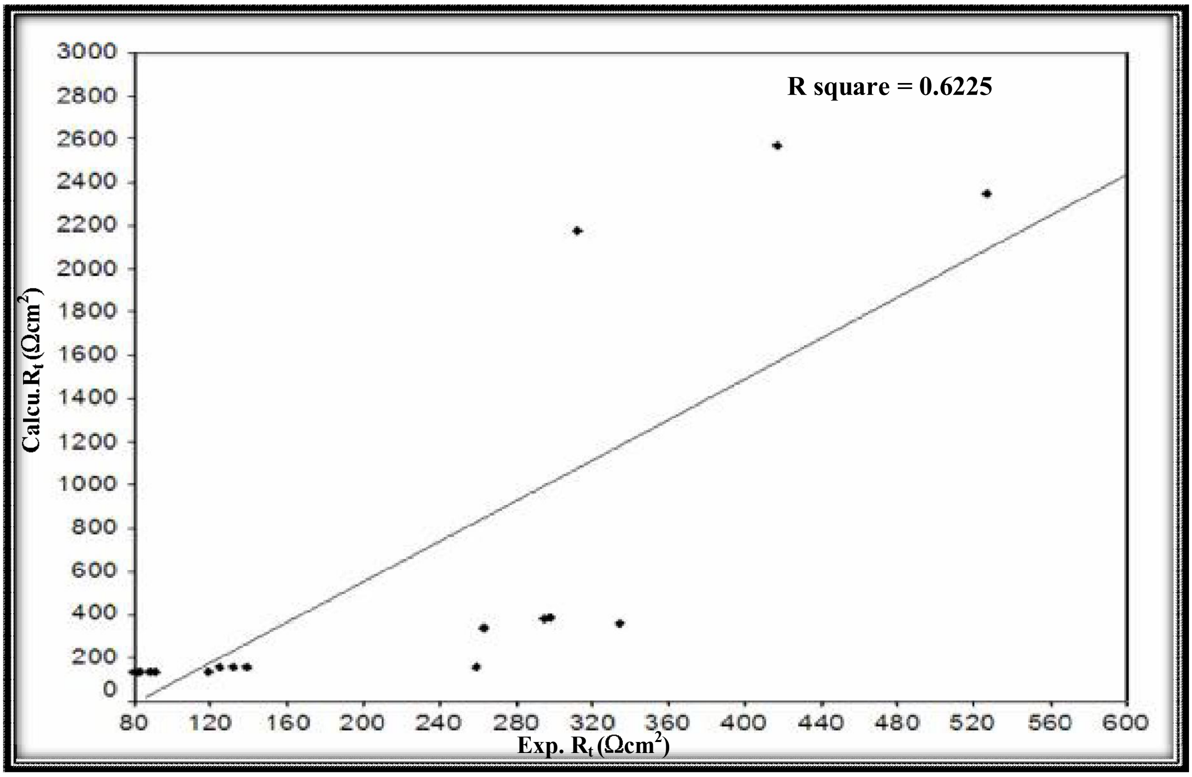


Fig.(1) : Experimental and calculated R_t values of pyrimidine inhibitor for first group by using the regression equation three.

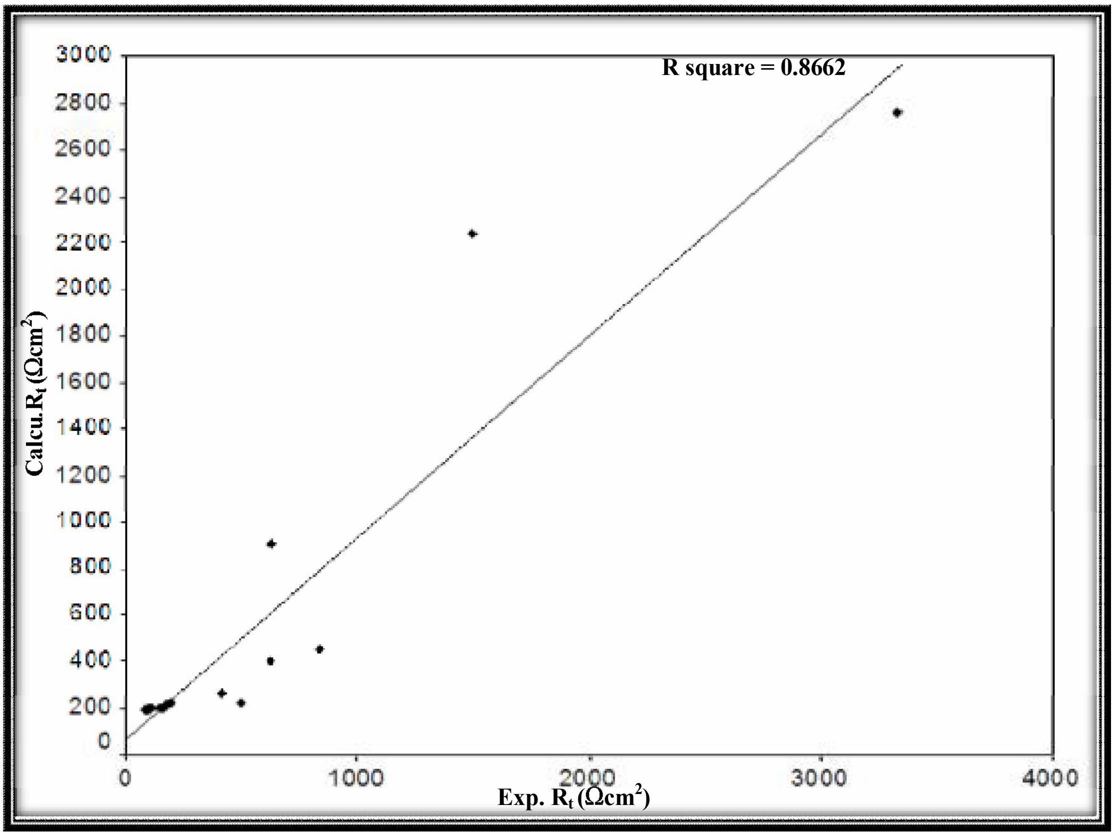


Fig.(2) : Experimental and calculated R_t values of pyrimidine inhibitor for second group by using the regression equation four.

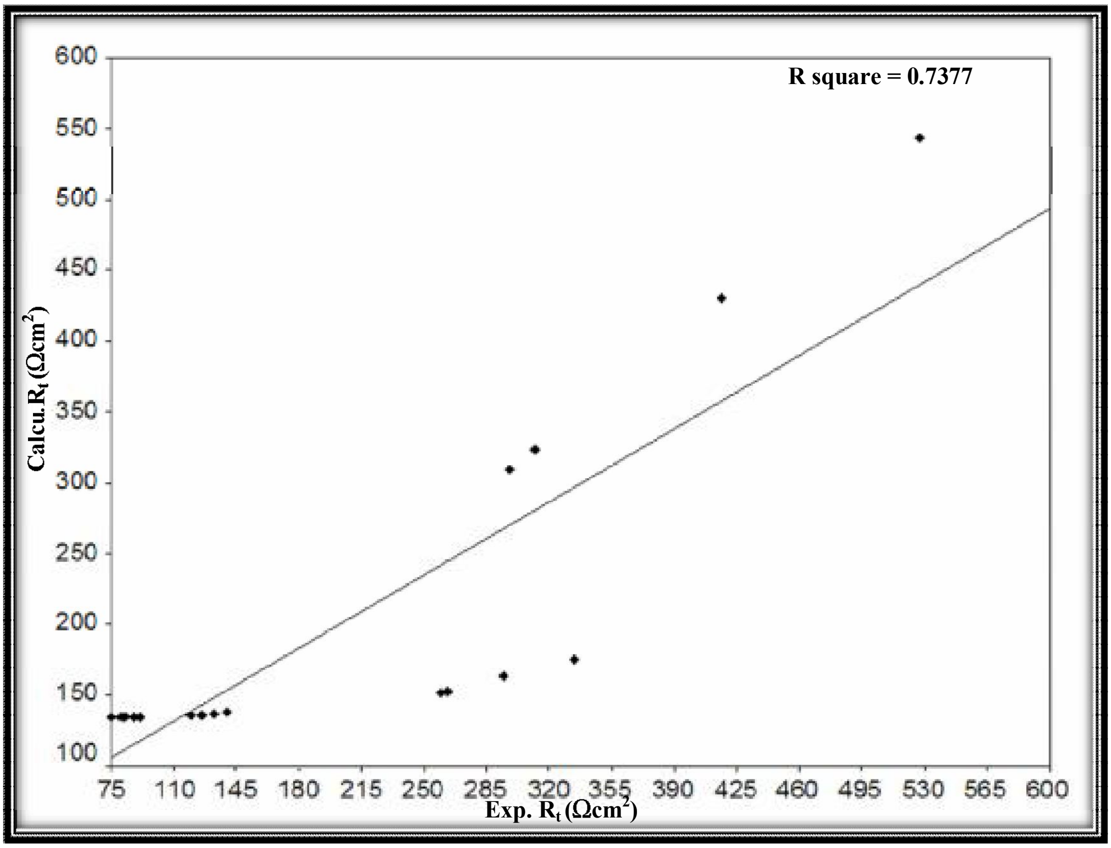


Fig.(3) : Experimental and calculated R_t values of pyrimidine inhibitor for first group by using the regression equation five.

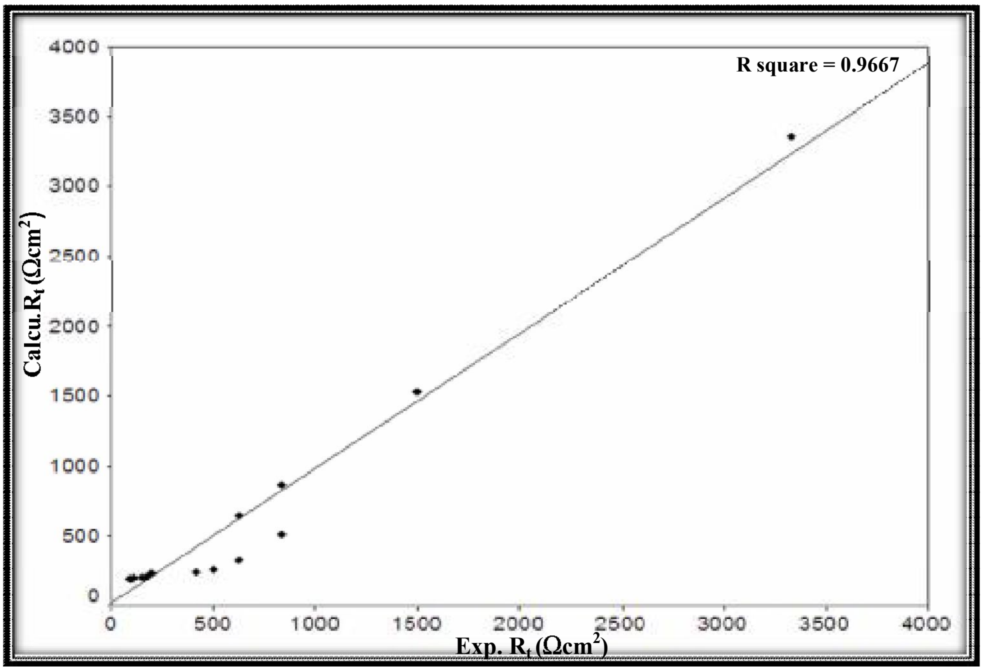
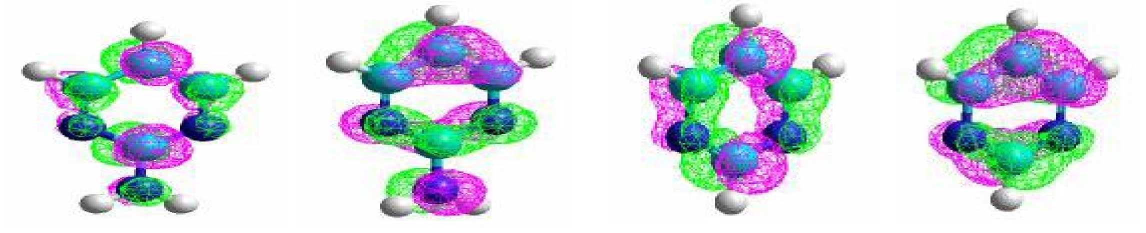
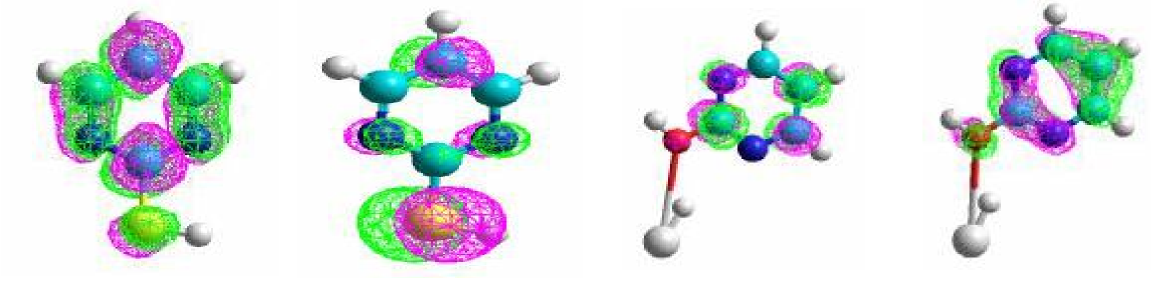


Fig.(4) : Experimental and calculated R_t values of pyrimidine inhibitor for second group by using the regression equation six.



2-methylprimidine
LUMO HOMO

Pyrimidine
LUMO HOMO



2-mercaptopyrimidine
LUMO HOMO

2-hydroxypyrimidinehydrochloride
LUMO HOMO

2,4,6-triaminopyrimidine
LUMO HOMO

2,4-diaminopyrimidine
LUMO HOMO

2,4-diamino-6-meracaptopyrimidine
LUMO HOMO

2,4-diamino-6-hydroxypyrimidine
LUMO HOMO

Fig. (5) : Molecular structure and HOMO, LUMO of pyrimidine inhibitors.

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الخلاصة

الحساباتِ الكيميائيةِ الكَمّيةِ أنجزت على مركب البريميدين ومشتقاتهُ التي تستخدم في العادة كمثبطات تآكل لقطب الحديد. باستخدام الطرق الشبة التجريبية المتمثلة بأنموذج أوستن. حُسبت طاقة أعلى مدار جزيئي مشغول و طاقة أوطأ مدار جزيئي غير مشغول إضافةً إلى حساب العزم ذو القطبين و الطاقات الالكترونية للجزيئات المدروسة . تقييم المثبط من الناحية الكيميائيةِ الكَمّيةِ والقيم العملية لكفاءة تثبيط المثبط نُفذَا للتحري عن أي صلات واضحة تَجِدُ بين نَتائِجِ الحساباتِ الكيميائيةِ الكَمّيةِ وكفاءاتِ المثبطات العملية المستخدمة لمركب البريميدين ومشتقاتهُ باستخدام الأنموذج الخطي المعتمد على مقاومة انتقال الشحنة. معاملات الترابط لمعادلات الانحدار المشتقة بين مقاومة انتقال الشحنة والحسابات الجزيئية كانت أكثر وثوق. وضوح معنوية الترابط يشير إلى تباين تثبيط التآكل للمادة المثبطة مع التركيب الجزيئي قَدْ يُوضّحُ من ناحية الخواص الإلكترونيةِ.