



## EXPERIMENTAL AND THEORETICAL STUDY OF 3-BENZYL -2-MERCAPTOQUINOIZOLINE-4(3H)-ONE (BMQ) AS AN INHIBITOR OF CARBON STEEL CORROSION IN ACIDIC MEDIA

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### ABSTRACT

The inhibition of 3-Benzyl -2-mercaptoquinoizoline -4 (3H)-one (BMQ) on the corrosion of carbon steel in 0.5 M HCl studied by potentiation polarization methods at 303–333 K. Results obtained show that BMQ act as inhibitor for carbon steel in HCl solution. The inhibition efficiency increase with increase in BMQ concentration. Activation parameters and Gibbs free energy for the adsorption process using Statistical Physics calculated and discussed. Quantum chemical calculations using DFT at the B3LYP/6-31G level of theory were used to calculate some electronic properties of the molecule to verify any correlation between the inhibitive effect and molecular structure of BMQ. The quantum calculations were proceeded to get data around correlation amid the BMQ and electronic structures of examined inhibitor and their trial corrosion inhibition efficiencies. The structural data, as  $E_{\text{HOMO}}$  (highest occupied molecular orbital energy),  $E_{\text{LUMO}}$  (lowest unoccupied molecular orbital energy) and dipole moment ( $\mu$ ),  $E$  is energy gap, the charge distribution, is absolute hardness and softness,  $N$  is number of electrons moved from BMQ to the surface of metal, as well as some electronic parameters, calculated and discussed to understanding the process of corrosion inhibition.

**KEYWORDS:** DFT, potentiation polarization, carbon steel, inhibitor, corrosion inhibition.

### INTRODUCTION

The growth of corrosion inhibitors founded on organic compounds including atoms of nitrogen, oxygen, sulfur, and numerous bonds in the molecules that facilitate adsorption on the surface of metal<sup>[1]</sup>. Across propensity to constitute a powerful coordination bond, which should increase the inhibition efficiency in arrangement:  $O < N < S$ <sup>[2]</sup>. The inhibitor containing N- had functions greater efficiently in HCl, than the inhibitor containing S- in  $H_2SO_4$ <sup>[3]</sup>. Moreover, the inhibitor which have both N and S atoms at the same time always demonstrate greater inhibition administration than that have single N or S atom. The corrosion inhibition efficiency of organic compounds is connected to their adsorption characteristic. Adsorption to rely on the type and the a condition of the metal surface, on the kind of corroded midst and the chemical a structure of inhibitor<sup>[1]</sup>. investigation analysis a formal account that the adsorption of corrosion inhibitors most importantly rely on several physicochemical characteristic of molecule, having a relationship to its active groups, to possible steric effects and electronic density of donor atoms; adsorption is assume also to rely on probable interaction of p-orbitals of the inhibitor with the d- orbitals of atoms surface, which result a great adsorption of inhibitor molecules on carbon steel surface, leading to the structure of a corrosion defending thin layer<sup>[4,5]</sup>. Acid solutions excessively which was industry used, chemical cleaning, pickling and desalting which to guide a corrosive attack. Consequently, exhaustion of the corrosion inhibitors to lower corrosion has raised in recent Years. The corrosion command by corrosion inhibitors is one of most ordinary, operative and economical methods

to preserve carbon steel in acid media<sup>[6,7]</sup>. Greatest number of famous corrosion inhibitors is organic compounds comprising hetero atoms, like O<sub>2</sub>, sulfur or nitrogen and multiplex bonds, whichever permit an adsorption on carbon steel<sup>[8]</sup>. It has noticed that adsorption of these corrosion inhibitors rely on physico-chemical a special characteristic of functional groups and electron density at the donor atom. The adsorption happen because of reaction in lone pair and p- orbitals of the corrosion inhibitor with d-orbitals of atoms surface on carbon steel, whichever evokes a larger adsorption of the corrosion inhibitor molecules on the metal surface, resulting to formation of a corrosion defense film<sup>[9-11]</sup>. The adsorption as well affected depending on construction and the charge of the surface of metal, and testing electrolyte character<sup>[12-16]</sup>. organic compounds with a large number were studied as corrosion inhibitors for iron and low alloyed steels<sup>[17-19]</sup>.

### EXPERIMENTAL

#### Materials and solutions

The corrosion inhibitors 3-Benzyl-2-mercaptoquinoizoline -4 (3H)-one (BMQ) was synthesized by the following procedure<sup>[20]</sup> and the structure of (BMQ) shown in Fig (1). The experiment was combination on a recently sheet which prepared of carbon steel of the following constitution (wt. %): 0.252 % Mn, 0.086 % C, 0.016 % S, 0.003 % P, and the remainder used Fe. The prepared metal sample, cleaned and degreased as formerly qualified<sup>[21]</sup>. This sample was successively smoothed with girdle crushing polishing machine, refined with sandpaper with various grit (80, 150, 220, 240, 320, 400, 1000, 1200 and

2000) with concatenation. Later than the smoothing a specimen was rinsed with distilled water, acetone in the end desiccated and sheltered a desiccator. Solutions with 0.5 M HCl prepared using dilution of analytic rank 37% HCl by distilled water. The concentration range of BMQ prepared then used (100-250 ppm).

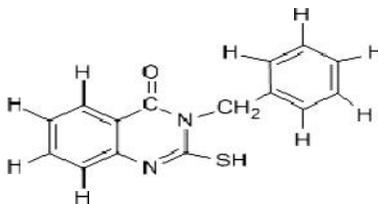


FIGURE 1: Structure of (BMQ).

### Corrosion study

The Potentiostatic polarization measurement was carried out using advanced Potentiostatic polarization model accomplished in a representative three-compartment glass cell comprised of the carbon steel sample as working electrode, platinum counting instrument electrode and a saturated calomel electrode such as the manual electrode. Wenking MLab-200 of Bank Elektronik-Intelligent controlled GmbH (Germany) and jacketed Pyrex glass cell. Polarization diagrams registered at fixed sweep rate of 2 mV/s and range of scanning from (-200 to +200 mV) with respect to open circuit potential. Before each experiment, the working electrode was covered with water in test cell for 30 min in order to reach invariable case condition. Each experiments were performed out at invariable temperature (through  $\pm 1^\circ\text{C}$ ) using governing cell temperature using a cooling-heating current water bath. Fascinated by variation automatically the electrode potential from -200 mV to +200mV against OCP with a scan rate of  $2.0 \text{ mVs}^{-1}$ . Every testing were be based on at a various concentration (100-250ppm) and at variant

temperature (303-333°k) tested. Tafel graphs of potential against log<sub>10</sub> plotted and the density of corrosion current ( $I_{\text{corr}}$ ) and the potential of corrosion ( $E_{\text{corr}}$ ) computed in presence and absence of corrosion inhibitor.

### Theoretical Computational calculation programs

The molecular of BMQ was to mark on a chart by Gaussian 03program; all quantum calculations were done using (DFT) Density Functional Theory at B3LYP/6-31G. overall optimizations of examined corrosion inhibitors done using density functional theory DFT by Beck's three parameter replacement functional together with Lee-Yang-Parr nonlocal relationship functional (B3LYP)<sup>[22-24]</sup> by 6-31G\* basis set applied by Gaussian 03 program package<sup>[25]</sup>. The contiguity indicated to profit approving geometries for a great width assortment of the systems. The 6-31G\* basis set which adopted gives perfect optimizations. The geometrical figure to make optimal without constraint. The subsequent quantum data were computed from received optimized construction ( $E_{\text{HOMO}}$ ) and ( $E_{\text{LUMO}}$ ), the energy gap ( $E$ ) between  $E_{\text{HOMO}}$  and  $E_{\text{LUMO}}$ , ( $\mu$ ) dipole moment, ( $\chi$ ) electronegativity, ( $A$ ) electron affinity, ( $\eta$ ) global hardness, ( $S$ ) softness, ( $I$ ) ionization potential, the global electrophilicity ( $\omega$ ) and ( $N$ ) is fraction of electrons transferred.

## RESULTS & DISCUSSION

### The effect of the BMQ corrosion inhibitor Concentration

The plotted curves for the corrosion inhibitors of metal surface in 0.5M HCl solution of Potentiostatic Polarization in presence and absence of BMQ (100-250 ppm) at 303-333°K as such illustrated in Figure (2). A linear area observed toward obvious Tafel, the activation of cathodic reaction repressed, the addition of the compound decreased the densities of the current in a great extent of anodic and cathodic potential field.

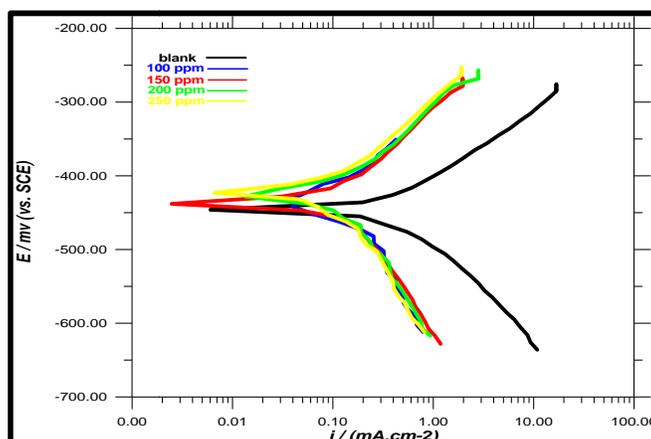


FIGURE 2: The curves of carbon steel Polarization in 0.5 M HCl in the absence and presence of [100-250 ppm] BMQ at 308 K.

The alteration in potentials may be a result of the rivalry of cathodic and anodic reactions of inhibiting, and the condition of surface metal<sup>[26]</sup>. The values of different electrochemical data are summarized in table 1. (% IE) is the percentage inhibition efficiency value, ( $\theta$ ) is coverage surface parameter, which described the part of covered

surface with the molecules of inhibitors, for metal surface corrosion was estimated by the following relation<sup>[27]</sup>:

$$\% IE = \frac{I_{\text{corr}} - I_{\text{corr}}(i_{\text{b}})}{I_{\text{corr}}} \times 100 \quad \text{-----1}$$

$$\Theta = \frac{I_{\text{corr}} - I_{\text{corr}}(i_{\text{b}})}{I_{\text{corr}}} \quad \text{-----2}$$

Icorr (inh) and Icorr are the corrosion currents densities in presence and absence of corrosion inhibitor, consecutively which estimated with extrapolation of anodic and cathodic Tafel lines (Ecorr) corrosion potential. From table1, it clarify that cathodic slope was established resembling pointing out that hydrogen reduction did not modify in existence of inhibitor. Presence (100-250 ppm) of BMQ leads to make values of Icorr smaller, which was especially important in case of BMQ the corrosion inhibitor experienced. Subsequently, the presence (100-250ppm) of BMQ leads to decrease the importance of Icorr, which especially important in case of BMQ. From

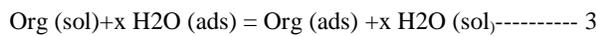
the outcome in Table 6, we clarify that rate of corrosion decreased by increasing the concentration of inhibitor, the inhibition efficiency increased in acid media as define in Figure (4). Consequently, the corrosion by mere obstruction the reaction location on surface of carbon steels without interferer the reactions of anodic and cathodic. Furthermore, the inhibitor reason no important changes in anodic and cathodic Tafel slopes, this suggest that the inhibitor act in particular way like avarious - sort inhibitor. Pointing out the inhibitor be able to sorted like adsorptive- sort<sup>[28]</sup>.

**TABLE 1:** The parameters of polarization of carbon steel in 0.5M HCl in presence and absence of (100,150,200,250) ppm of BMQat 303 K

C	E <sub>corr</sub>	I <sub>Corr.</sub>	β <sub>a</sub>	β <sub>c</sub>	W.L.	P.L.	I.E.	Θ
β	-427.200	135.700	-141.600	77.700	3.390	1.500	----	-----
100	-416.700	61.010	-177.000	97.000	1.530	7.08	54.520	0.455
150	-432.700	59.620	-124.000	117.400	1.490	6.910	56.140	0.561
200	-419.600	56.620	-169.000	108.100	1.420	6.570	58.28	0.582
250	-398.600	46.040	-173.200	87.900	1.150	5.340	66.070	0.660

**Adsorption isotherms& Thermodynamic parameters of adsorption**

Usually considered that adsorption of inhibitors on metal surface is fundamental step in inhibition mechanism<sup>[29]</sup>. The coverage surface (θ) supposed that inhibitor efficiency is due excessively to the hindering effect of adsorbed species. Fundamental data on interaction between metal surface and inhibitor scan be supplying by isotherms of adsorption<sup>[30]</sup>. Adsorption can occur of organic adsorb ate at metal solution interface as a consequence of displacement process adsorption between water molecules and organic molecules in the aqueous solution (Org (sol)), before adsorbed on surface of metal (H<sub>2</sub>O<sub>(ads)</sub>)<sup>[31]</sup>:

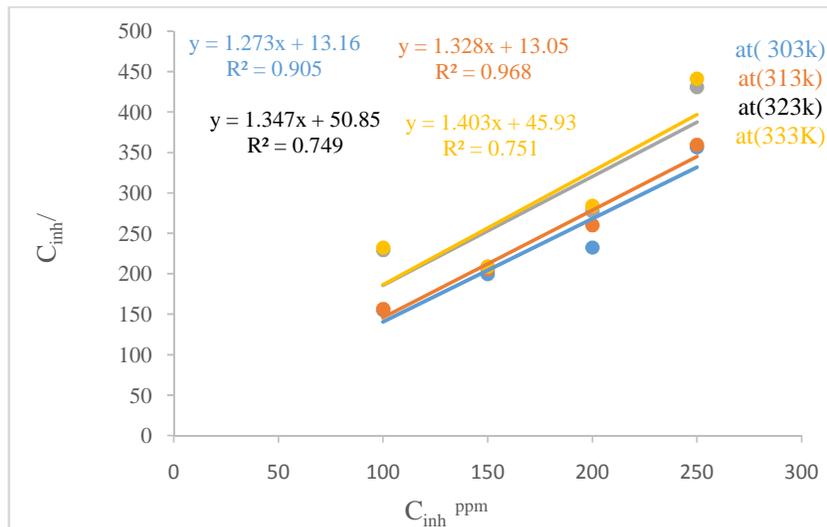


The greater part of solution the Org (sol) and Org (ads) are organic type and adsorbed one on the surface of metallic,

consecutivelythe water molecule numberis H<sub>2</sub>O (ads) adsorbed on thesurface of metallic and the extent ratio is x exemplification the number molecules of water substituted through one organic adsorbate. So that, to get isotherm of adsorption, θ is covering surface, the different concentrations for inhibitor in 0.5 M HCl solution had been estimated using equation (2). The values of θ that offered in Table (2). Depending on Langmuir’s isotherm, θ is surface coverage correlated with concentration of inhibitor (C) according to following equation<sup>[32]</sup>:

C / θ = (1/ K<sub>ads.</sub>) + C -----4

The equilibrium constant is K<sub>ads</sub> of process of adsorption, we obtained straight line by plotting C/θ versus C as illustrated in Figure (3).



**FIGURE 3:** The Langmuir adsorption isotherm for carbon steel in 0.5M HCl in various concentrations of (BMQ) inhibitor at (303-333) °K.

The ( $R^2$ ) is linear correlation coefficient is nearly equalize to ( $R^2 = 0.9980$ ), slope is approach 1, pointing out to inhibitor adsorption (BMQ) onto surface of Carbon steel submit to isotherm of Langmuir adsorption.

**TABLE 2:** Data of surface coverage and data of adsorption isotherm for metal surface at 0.5M HCl solution with various concentrations of BMQ inhibitor in (303-333)° K.

T(°K)	1/T(°K <sup>-1</sup> )	C (ppm)	Θ	C / Θ	K <sub>ads</sub> (M <sup>-1</sup> )	R <sup>2</sup>
303	0.0033	100	0.6603	0.4552	6.3613	0.9890
				0.5610		
				0.5820		
				0.6600		
				0.5294		
313	0.0032	150	0.6954	0.5950	3.4094	0.9980
				0.5630		
				0.6950		
				0.6550		
				0.6900		
323	0.0031	200	0.7392	0.7250	0.84331	0.9960
				0.7390		
				0.5011		
				0.6720		
				0.7081		
333	0.0030	250	0.7226	0.7220	1.07631	0.9950

The factor ( $R^2$ ) high relationship of Langmuir adsorption isotherm. The ( $K_{ads}$ ) the constant of equilibrium for adsorption and desorption process of examined inhibitor computed from multiplicative inverse of intercept. The ( $K_{ads}$ ) is equilibrium constant, adsorption evaluate in Table (2) were enumerated. Data in Table (2) also exposed that ( $K_{ads}$ ) adsorptive equilibrium constant in the temperature range 303–333 °K increase slightly. ( $G_{ads}$ ) the adsorption free energy calculated at various temperatures from sequent equation<sup>[33]</sup>:

$$G_{ads} = - 2.303 RT \log ( 55.5 K_{ads} ) \text{ ----- } 5$$

(R) is a gas constant, the absolute temperature is T, and 55.5 is the water concentration value in solution of declared by ppm, the equilibrium constant  $K_{ads}$  for process of inhibitor adsorption.  $G_{ads}$  Values listed in Table (3). The values are usually characteristic of  $G_{ads}$  negative sign of powerful interaction and a high competent adsorption. Usually,  $G_{ads}$  values about (-10.3299) kJ mol<sup>-1</sup> or lower negative are compatible with electrostatic interaction between the molecules charged and metal charged. Since values which much negative values than -10.3299kJ mol<sup>-1</sup> include charge participation or transportation from the molecules of inhibitor to surface of metal to mold a coordinate kind of bond (chemisorption)

<sup>[34]</sup>. Computed values of  $G_{ads}$  show the mechanics of adsorption of affected inhibitor on surface of metal in 0.5M HCl Solution is chemical adsorption. From a chart of log  $K_{ads}$  vs. 1/ T, ( $H_{ads}$ ) the adsorption heat, which taken of slope of the linear part of curve, is equalize to -  $H_{ads} / 2.303R$ . The  $H_{ads}$  value of synthetic inhibitor is equal to -51.6220 kJ mol<sup>-1</sup>. The  $H_{ads}$  value with negative sign to point out that adsorption of investigated inhibitor on surface of carbon steel is exothermic. When ( $H_{ads}$  less than 0) process is an exothermic adsorption be possible assigned as chemisorption<sup>[35]</sup>. The exothermic reaction, chemisorption is able to characteristic according to estimation  $H_{ads}$  the absolute value. The physisorption,  $H_{ads}$  is less than 40 kJ.mol<sup>-1</sup> while the chemisorption,  $H_{ads}$  contiguity 100 kJ.mol<sup>-1</sup><sup>[36]</sup>. ( $S_{ads}$ ) the entropy of inhibitor adsorption is computed by the sequent equation<sup>[37]</sup>:

$$G_{ads} = H_{ads} - T S_{ads} \text{ ----- } 6$$

Values of  $S_{ads}$  illustrated in table (3). It monitored the  $S_{ads}$  values in the existence of inhibitor with negative sign values, which clarified a decrease of disorder is result to the adsorption of one molecule of inhibitor according to desorption of low water molecules<sup>[38]</sup>.

**TABLE 3:** The thermodynamic data of adsorption inhibitor BMQ at various concentrations on carbon steel in HCl solution with 0.5M.

T (K°)	G <sub>ads</sub> (kJ/mol)	H <sub>ads</sub> (kJ/mol)	S <sub>ads</sub> (J/mol.K)
303	-14.7815	-51.6220	-121.588
313	-13.6461	-51.6220	-121.331
323	-10.3299	-51.6220	-127.841
333	-11.3252	-51.6220	-121.013

**The effect of temperature**

The temperature is an essential data in investigation on metal dissolution studies<sup>[39]</sup>. The rate of corrosion in acid solutions increases with temperature increase

exponentially due to the hydrogen development over potential decreases<sup>[40]</sup>. For investigate the mechanism of inhibition and to estimate the activation energy  $E_a$  of corrosion process, curves of polarization of carbon steel in

0.5 M HCl concentration range (100-250) ppm of BMQ inhibitor. Check Table (4), to show that the rate of corrosion decreases and consequently I.E% increases as temperature increases figure (4). Explain that the rising of temperature increases the inhibition and the highest

inhibition efficiency is taken with (250 ppm) (BMQ) at (323) K. in case of (150 ppm) the inhibition efficiency decrease at (313) K because of control of desorption process more than adsorption<sup>[41]</sup>.

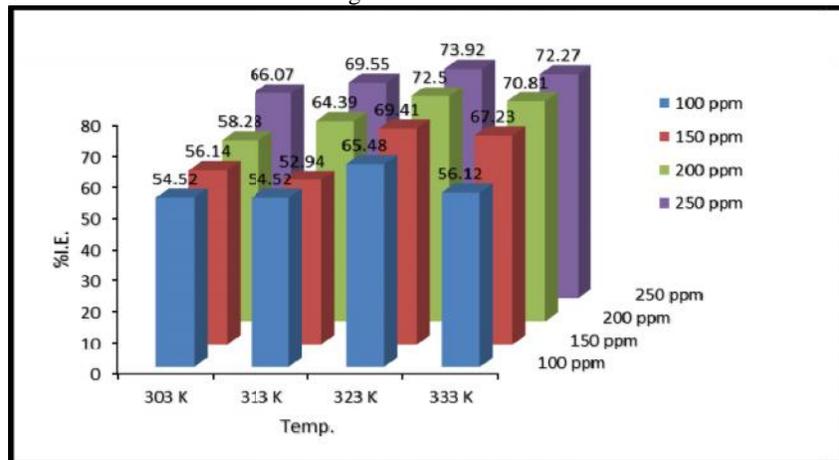


FIGURE 4: The correlation between inhibition efficiencies with various temperature (303-333) °K of carbon steel in 0.5M HCl of (BMQ) inhibitor in various concentrations

TABLE 4: The influence of temperature on corrosion data of carbon steel in 0.5 M HCl with various concentrations with (BMQ) inhibitor

T(K)	C	E <sub>cor</sub>	I <sub>Cor.</sub>	B <sub>a</sub>	B <sub>c</sub>	W.L.	P.L.	%I.E.	Θ
303	B	-427.200	135.700	-141.600	77.700	3.390	1.500	----	-----
	100	-416.700	61.010	-177.000	97.000	1.530	7.08	54.520	0.455
	150	-432.700	59.620	-124.000	117.400	1.490	6.910	56.140	0.561
	200	-419.600	56.620	-169.000	108.100	1.420	6.570	58.28	0.582
	250	-398.600	46.040	-173.200	87.900	1.150	5.340	66.070	0.660
313	B	-441.500	182.840	-104.500	78.500	4.500	2.120	----	-----
	100	-436.200	86.030	-160.000	111.100	2.150	9.900	54.520	0.529
	150	-427.200	73.960	-177.900	115.100	2.220	1.030	52.940	0.595
	200	-428.000	65.110	-117.000	98.500	1.630	7.560	64.390	0.563
	250	-405.000	55.680	-141.700	96.200	1.390	6.460	69.550	0.695
323	B	-446.300	288.820	-95.500	84.300	7.220	3.350	----	-----
	100	-432.900	99.710	-136.000	130.300	2.490	1.160	65.480	0.654
	150	-437.900	88.360	-124.800	116.100	2.210	1.030	69.410	0.690
	200	-428.300	79.420	-130.500	102.100	1.990	9.220	72.500	0.725
	250	-422.000	75.310	-148.400	107.000	1.880	8.740	73.920	0.739
333	B	-448.200	319.060	-94.300	74.100	7.980	3.700	----	-----
	100	-436.000	140.000	-172.000	105.900	3.500	3.500	56.120	0.561
	150	-428.000	104.600	-135.500	108.000	2.610	1.210	67.230	0.672
	200	-434.400	93.120	-114.400	117.800	2.330	1.080	70.810	0.708
	250	-432.400	88.480	-137.600	103.400	2.210	1.630	72.270	0.722

The (Ea) values of activation energy computed from modified Arrhenius equation<sup>[42]</sup>:

$$\text{Log } i_{\text{corr.}} = \text{LogA} - \text{Ea} / (2.303 \text{ RT}) \text{-----(7)}$$

Where  $i_{\text{corr}}$  is corrosion current density, **Ea** is obvious activation energy of corrosion process, R is the gas constant, T is absolute temperature and A is factor of Arrhenius pre-exponential. Figure (5) give the Arrhenius chart of natural logarithm of current density vs 1/T, the 0.5M HCl solution, with and without various concentrations of (BMQ) inhibitor evaluate of A and Ea for corrosion process are computed with a linear regression technique as granted in table 5. It available that activation energy is more in presence of inhibitor than in its absence of inhibitor.

Ea proportion venatic with synthesized inhibitor BMQ concentration. Its become clarified that concentration of inhibitor (BMQ) is representing in growing the value of activation energy, because of that pointing out a greater effect of efficient inhibiting. The increase in inhibiting efficiency with inhibitor concentration is exemplary of chemisorption process<sup>[43]</sup>. This was assigned by Holliday and Hoar<sup>[44]</sup> to a low rate of inhibitor adsorption with a consequent nearer contiguity to equilibrium within experiments at maximum temperature. However, Hurd and Riggs<sup>[45]</sup> clarified that the increase in the **Ea** of corrosion at a maximum position of inhibition result from a shift of the net corrosion process of discovered part of metal surface to wrapped one. Huang and Schmid<sup>[46]</sup> discover that organic molecules inhibit both the cathodic and anodic fractional reactions on electrode surface and a

resembling reaction occur in the wrapped area, but the rate of the reaction on wrapped area is more than on the unwrapped area like that in this research table (5). Depending on eq. (7), great values of A and low values of

$E_a$  cause to higher rates of corrosion. For present research,  $E_a$  is lower in presence of BMQ. Consequently, the decrease in rate corrosion is intelligible with (A) pre-exponential factor.

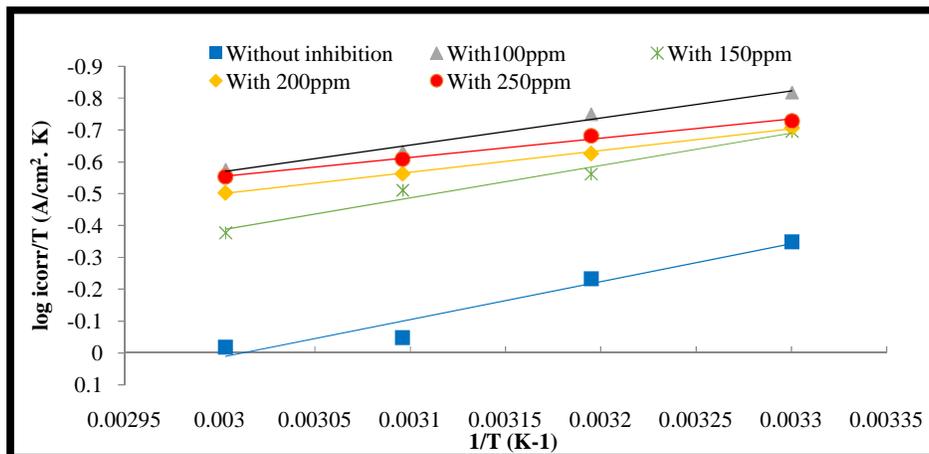


FIGURE 5: Arrhenius diagram between  $\log i_{corr}$  against  $1/T$  with and without of various concentrations of (BMQ) inhibitor

TABLE 5: Thermodynamic parameters to activation of corrosion inhibitor BMQ in variant concentrations of carbon steel in 0.5M HCl

C (ppm)	A(A/cm <sup>2</sup> )	Ea(KJ/mol)
	2.00954	25.42740
100	2.43300	22.13409
150	1.82766	15.68940
200	9.30670	14.17080
250	5.06100	18.95180

### Theoretical Results and discussion of BMQ

The computational accounts were proceeded to get data about correlation between BMQ and electronic building of examined inhibitor and their trial efficiencies of corrosion inhibition. The constructional data, like the energy of highest occupied molecular orbital  $E_{HOMO}$ ,  $E_{LUMO}$  the energy of lowest unoccupied molecular orbital, ( $\mu$ ) dipole moment, energy gap  $E = E_{LUMO} - E_{HOMO}$ , the charge distribution, the absolute hardness, softness and  $N$  is number of electrons transferred from BMQ to metallic surface by Density Functional Theory at B3LYP/6-31G, as well as some electronic parameters calculated and discussed to understanding the process of corrosion inhibition. The results showed that the efficiency of

corrosion inhibition increased at increase the values of highest occupied molecular orbital energy but decreased at a decrease in the energy of lowest unoccupied molecular orbital value<sup>[47]</sup>. Hence, increasing data of  $E_{HOMO}$  suggest a greater orientation t donation the electron (s) to adequate receiver molecule having low energy that have an empty molecular orbital<sup>[48]</sup>. The ( $\mu$ ) is an evaluate of apolarity in the bond and is connected with the electrons distribution in the molecule. The dipole moment was another indicator of electronic distribution within a molecule<sup>[49]</sup>. The Mulliken charge distribution of the inhibitor could readily observed in Figure (6). That S, O, N and somewhat carbon atoms have great charge densities are effective centers, which have the strongest capability to bond to metal surface<sup>[50]</sup>.

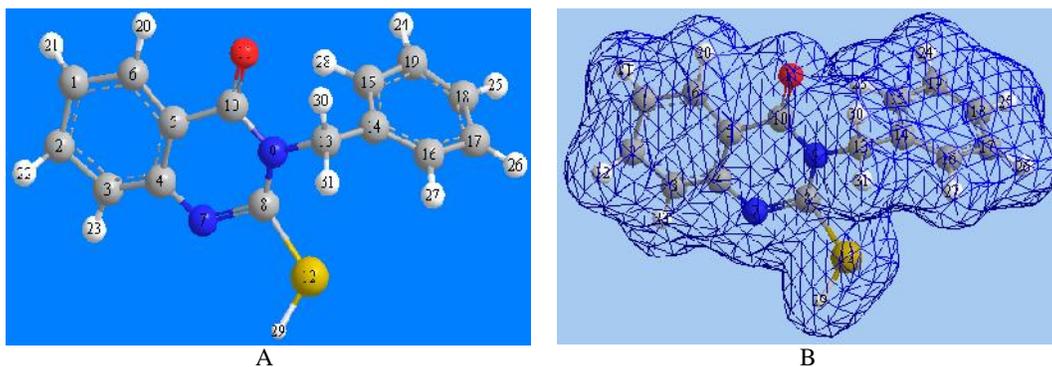
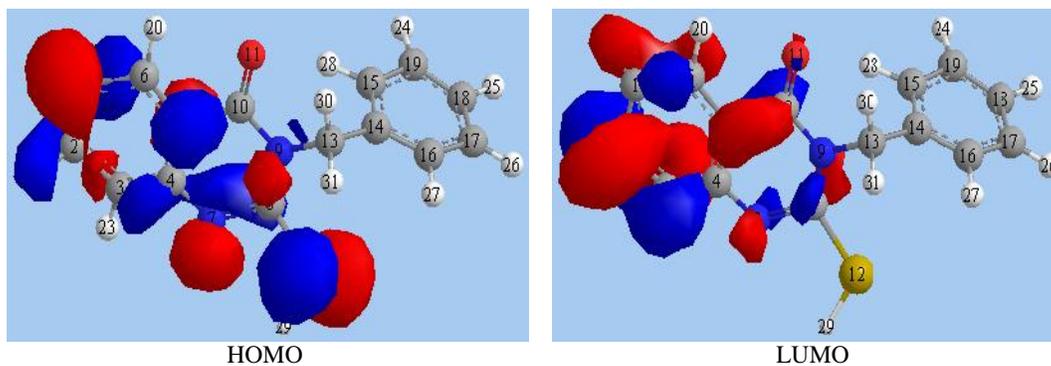


FIGURE 6: A-The Optimized structure of BMQ, B- Mulliken charges distribution of BMQ inhibitor by Density Functional Theory

The sequent quantum calculations evidence: the ( $E_{HOMO}$ ), the ( $E_{LUMO}$ ), energy gap and ( $\mu$ ). Figure (7) explain the ( $E_{HOMO}$ )and the ( $E_{LUMO}$ ), of BMQ as corrosion inhibitor using Density Functional Theory at B3LYP/6-31G.



**FIGURE 7:** The ( $E_{HOMO}$ ) and ( $E_{LUMO}$ ), of BMQ as corrosion inhibitor using Density Functional Theory at B3LYP/6-31G

Whereas the inhibitors and Fe are jointly, the electrons will transfer of lower (inhibitor) to higher (Fe) with balancing the chemical potentials. like a first approximation, N the fraction of electron transferred<sup>[51]</sup>, is explicator in equation (8):

$$N = ( \chi_{Fe} - \chi_{inh} ) / 2 ( \chi_{Fe} + \chi_{inh} ) \text{-----} 8$$

Whither  $\chi_{Fe}$  and  $\chi_{inh}$  indicate to absolute electro negativity to Fe and corrosion inhibitor consecutively;  $\chi_{Fe}$  and  $\chi_{inh}$  exhibit for absolute hardness of Fe and BMQ as corrosion

inhibitor molecule, continually. From eq. (8), Fe is behave as Lewis acid in agreement with Hard and Soft Acid and Base theory (HSAB)<sup>[52]</sup>.The electron transfer due to the difference in electro negativity drives, and the total of hardness data perform like a resistance<sup>[51]</sup>. The amounts are clinging to the (A) electron affinity and (I) ionization potential which are practical in capability to help forecast chemical conduct<sup>[53]</sup>.

$$\begin{aligned} &= (I + A) / 2 \text{-----} 9 \\ &= (I - A) / 2 \text{-----} 10 \end{aligned}$$

**TABLE 6:** The molecular properties of BMQ computed by Density Functional Theory at B3LYP/6-31G

Molecular parameters	Calculated values
E(RB+HF-LYP) (au)	-1161.446
Dipole moment (D)	-5.568
$E_{HOMO}$ (eV)	-5.268
$E_{LUMO}$ (eV)	-2.160
E (eV)	3.408
I(eV)	5.268
A(eV)	2.160
$\mu = (I+A) / 2$	3.714
$\Delta N = (I-A) / 2$	1.554
N	1.057

I and A are connected in to  $E_{HOMO}$  and  $E_{LUMO}$  as follows:

$$I = - E_{HOMO} \text{-----} 11$$

$$A = - E_{LUMO} \text{-----} 12$$

The values of  $\chi$  and  $\mu$  computed using data of I and A taken from calculations of quantum mechanics. By theoretical value = 7 eV/mol depending on Pearson’s scale for electro-negativity<sup>[51]</sup> and  $\mu$  value a global hardness, and to Fe,  $M = 0$  eV/ mol with supposing to a metallic mass  $I = A^{[54]}$ , N, whichever recognition electrons fraction moved from inhibitor to metal surface of carbon steel was computed in table (6). The N data of studied inhibition affective consequence of electrons donation. In agreement with<sup>[55,56]</sup>, whether  $N < 3.6$ , inhibition efficiency raised with raising donating electron capability at metal. In this research, BMQ electrons donator, and surface of carbon steel was receiver<sup>[57]</sup>. The

E gap of BMQ,  $E = E_{LUMO} - E_{HOMO}$ , is an important data that should be regarded<sup>[58]</sup>. Great values of E suggest high electronic durability to bring about low

reactivity when low values suggest that will be remove easier an electron from  $E_{HOMO}$  to  $E_{LUMO}$  orbital which can bring about high inhibition efficiency to BMQ. We can notice the increase in  $\mu$  values,  $\Delta N$  which show a high disposal to donate their electron of inhibitors; therefore occur a better adsorption on the surface of carbon steel<sup>[59]</sup>.

**CONCLUSION**

The inhibiting effect of BMQ in 0.5 M HCl on the surface of metal was investigated experimental and theoretical. We get good results and the chief conclusions as follows: BMQ was actual be the best inhibitor to carbon steel in 0.5M HCl. The efficiency of BMQ growing with increase of BMQ concentration. BMQ is being there in solution data of activation energy become smaller. Adsorption of BMQ on surface metal in 0.5M HCl obeys the isotherm of Langmuir adsorption and guide to the structure of a defensive film. The analyzing of trial data guides to proposal the process of inhibitor on the carbon steel was

chemisorptions. Actually, the corrosion activation energy is lower in BMQ presence than in absence.

Using Density Functional Theory at B3LYP/6-31G., the geometries of molecule and studied rustle leading to the next conclusions: The quantum chemical studied data are in excellent acceptance with experimental examinations. The effect obviously discovered in balancing with BMQ, and so in enhancement of the efficacy provide with addition of  $\mu$ ,  $\Delta N$  values and so by the  $\Delta E$ ,  $\eta$  values decreased.

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