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*by* Saprizal Hadisaputra

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## 2 Theoretical study on the corrosion inhibition performance of dibenzo-18-crown-6 and its derivatives

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**Abstract.** Theoretical studies on the performance of corrosion inhibition of dibenzo-18-crown-6 compounds and its derivatives have been carried out using the B3LYP/631G(d) theory level. The effect of electron donor groups (NH<sub>2</sub>, OCH<sub>3</sub>, OH, CH<sub>3</sub>, CHCH<sub>2</sub>) and electron withdrawing groups (COOCH<sub>3</sub>, COOH, CHO, F, NO<sub>2</sub>) was also studied in the gas and aqueous medium. Electron donor groups increase the value of corrosion inhibition efficiencies; in contrast electron withdrawing groups have the opposite effects. The theoretical calculation indicated that NH<sub>2</sub> gave the highest efficiency value, whereas the NO<sub>2</sub> group gave the lowest corrosion inhibitor efficiency value. The positive correlation was shown between the corrosion inhibition efficiency and the quantum parameters. The Fukui function showed that the delocalisation of electrons around the benzene ring was the area that most contributes to the bond formed between the metal and the crown ether.

### 5 1. Introduction

Corrosion is an inevitable electrochemical process for less noble metals and alloys. It gradually destroys structures when metals interact with a corrosive environment such as hydrochloric acid [1]. Having no prevention, corrosion may lead to massive economic losses. Therefore, intensive efforts to gain high-efficiency and the feasible use of the corrosion inhibitors are still a very active research area. Moreover, searching for less toxic and environment-friendly corrosion inhibitors becomes significantly important due to the increased awareness of the importance of the green chemistry applications. 2 variety of organic compounds has been used as green corrosion inhibitor [2-4]. The existence of electronegative functional groups such as heteroatomic oxygen, sulfur, nitrogen and  $\pi$ -electron are the conditions for inhibitors to have high efficiency [5-7]. This functional group helps molecules to be bound to metal surfaces to inhibit corrosion by chemisorption or physisorption [8,9]. The uniform films of organic molecules attached to the surface prevent metals from interacting with the corrosive medium [10].

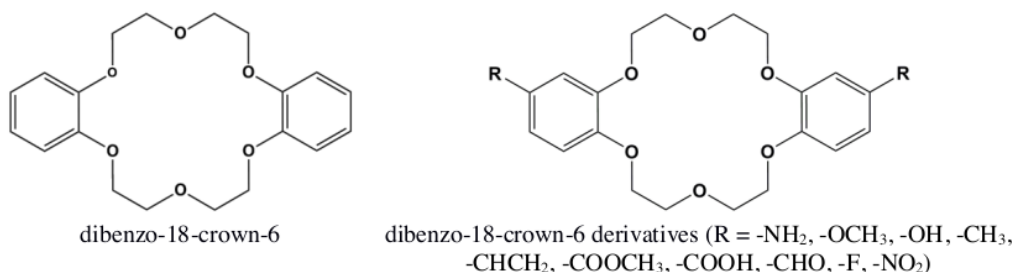
Many organic material-based corrosion inhibitors have been reported [11-13]. However, very few experimental studies have attempted to study the performance of crown ether compounds as corrosion inhibitors [14-15]. Furthermore, the theoretical studies have been used extensively for the study of crown ether with some metal ions [16-20]. The same approach is also widely used to study the effect of adding crown ether to the prevention of corrosion [21-22]. The structural properties of the crown ether can be easily modified to meet the corrosion inhibitor's criteria. Modification on the heteroatoms (O, N, and S), and adding the  $\pi$ -electron in multiple bonds such as benzene groups within the crown ether framework may change their corrosion inhibition performance. Furthermore, crown ethers are less toxic and environment-friendly which are suitable for green corrosion inhibitors. Fouda *et al.* [15] reported that the crown ethers are a highly potential candidate for corrosion inhibitors and those show good corrosion inhibitors efficiencies. This experimental work shows the different crown ether ring size and substituent types of corrosion inhibition of stainless steel by crown ether. In this current work, we use theoretical approach to determine the relationship between substituent effect and inhibition efficiency of the dibenzo-18-crown-6 and its derivatives.

## 2. Computational Method

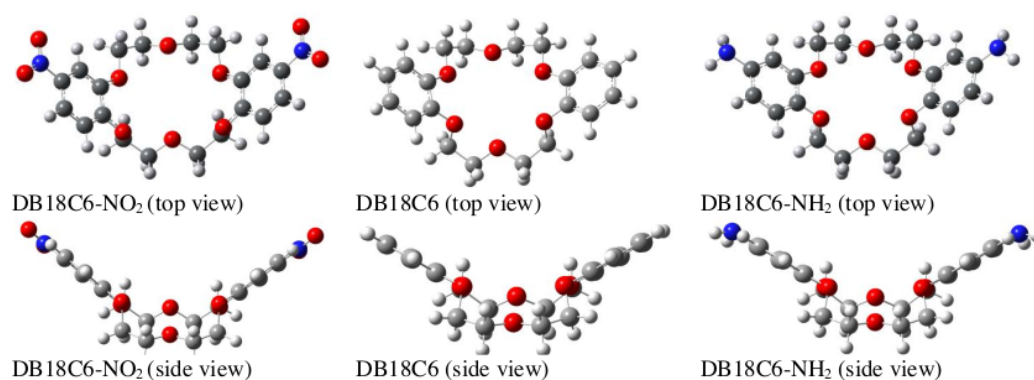
The density functional calculation at B3LYP/6-31G level of theory was used for geometry optimization from the studied crown ether. The Gaussian 03 package was applied to calculate all quantum parameters [23]. Optimization of crown ether geometry in the gas phase was carried out in the no symmetry constraint to reach the molecular ground state condition. The effect of the solvent was included using the PCM method to mimic the corrosion conditions in the aqueous environment. Re-optimization of the crown ether structure in the aqueous phase was not carried out because only gave a minor effect on the energetic. Therefore, the result of a single point calculation in the gas phase was sufficient to represent its energy [19-22].

## 3. Results and Discussion

Two different types of substituents were chosen as substituents of the corrosion inhibitor molecules, benzo-18-crown-6 (DB18C6), electron donating and electron withdrawing substituents. The series of electron-donating (R = -NH<sub>2</sub>, -OCH<sub>3</sub>, -H, -CH<sub>3</sub>, -CHCH<sub>2</sub>) and -withdrawing substituents (R = -COOCH<sub>3</sub>, -COOH, -CHO, -F, -NO<sub>2</sub>) were added into the benzo unit of dibenzo-18-crown-6 as depicted in Scheme 1. Figure 1 shows the structure of the optimized geometries of crown ethers (DB18C6-NO<sub>2</sub>, DB18C6 and DB18C6-NH<sub>2</sub>) calculated by DFT method. Figure 1 shows that the DB18C6 conformation undergoes very little change due to the addition of substituent groups. The presence of benzene on both sides of DB18C6 makes the molecule rigid so that the number of conformational isomers is small. Only conformational CSs are selected at the stage of geometry optimization and as a result, the computational effort is successfully reduced. The structural parameters of the studied crown ether can be seen in our previous publication [16].



**Scheme 1.** Structure of the studied dibenzo-18-crown-6 (DB18C6) and its derivatives



**Figure 1.** The optimized structures of the studied molecules (R= NO<sub>2</sub>, H, NH<sub>2</sub>) determined using DFT method.

**Table 1.** Quantum-chemical parameters for dibenzo-18-crown-6 (H) and eleven models determined using DFT method at gas (G) and solvent (W) phase

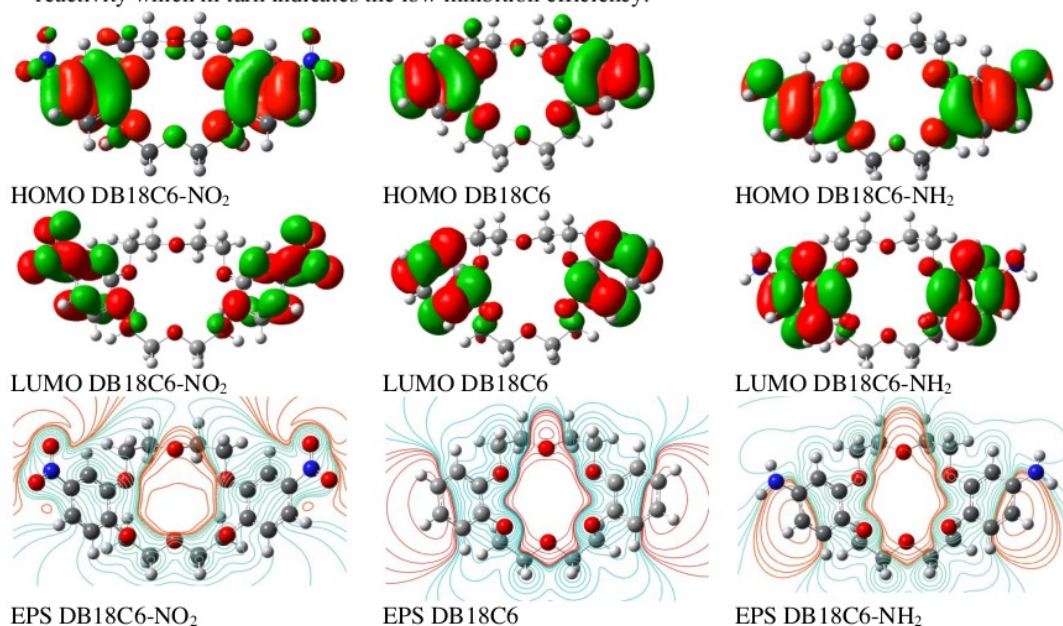
Substituents	Phase	E <sub>HOMO</sub> (eV)	E <sub>LUMO</sub> (eV)	E <sub>g</sub> (eV)	I (eV)	A (eV)	χ (eV)	η (eV)	σ (eV)	ΔN	IE <sub>theor.</sub> %
H	G	-5.5805	0.2242	5.8047	5.5805	-0.2242	2.6781	2.9023	0.3445	0.7445	
	W	-5.8793	-0.0299	5.8493	5.8792	0.0299	2.9546	2.9246	0.3419	0.6915	63.1300
CHCH <sub>2</sub>	G	-5.4765	-0.6982	4.7783	5.4765	0.6982	3.0874	2.3891	0.4185	0.8188	64.3059
	W	-5.7288	-0.9007	4.8281	5.7288	0.9006	3.3147	2.4140	0.4142	0.7632	64.7458
CH <sub>3</sub>	G	-5.4433	0.3191	5.7625	5.4433	-0.3191	2.5620	2.8812	0.3470	0.7701	64.6814
	W	-5.7767	0.0326	5.8093	5.7767	-0.0326	2.8720	2.9046	0.3442	0.7105	64.2315
OH	G	-5.2074	0.3504	5.5579	5.2074	-0.3504	2.4284	2.7789	0.3598	0.8225	67.3503
	W	-5.4901	0.1145	5.6047	5.4901	-0.1145	2.6878	2.8023	0.3568	0.7693	67.3082
OCH <sub>3</sub>	G	-5.1900	0.4160	5.6060	5.1900	-0.4160	2.3869	2.8030	0.3567	0.8228	67.5473
	W	-5.5884	0.1145	5.7029	5.5884	-0.1145	2.7369	2.8514	0.3506	0.7475	66.2534
NH <sub>2</sub>	G	-5.0934	0.4108	5.5043	5.0934	-0.4108	2.3412	2.7521	0.3633	0.8463	68.6401
	W	-5.3669	0.1463	5.5133	5.3669	-0.1464	2.6102	2.7566	0.3627	0.7962	68.6318
F	G	-5.7250	0.1017	5.8267	5.7250	-0.1017	2.8116	2.9133	0.3432	0.7188	61.4954
	W	-5.9236	-0.0544	5.8692	5.9236	0.0544	2.9890	2.9346	0.3407	0.6833	62.6537
COOCH <sub>3</sub>	G	-5.8417	-0.8857	4.9560	5.8417	0.8857	3.3637	2.4780	0.4035	0.7337	60.1748
	W	-6.1364	-1.2032	4.9331	6.1364	1.2032	3.6698	2.4665	0.4054	0.6750	60.3688
COCH <sub>3</sub>	G	-5.9073	-1.2345	4.6727	5.9073	1.2345	3.5709	2.3363	0.4280	0.7338	59.4329
	W	-6.1467	-1.5102	4.6365	6.1467	1.5102	3.8285	2.3182	0.4313	0.6840	60.2578
COOH	G	-5.9541	-1.0748	4.8792	5.9541	1.0748	3.5144	2.4396	0.4098	0.7143	58.9034
	W	-6.1451	-1.2217	4.9233	6.1451	1.2217	3.6834	2.4616	0.4062	0.6736	60.2753
CHO	G	-6.0678	-1.4849	4.5829	6.0678	1.4849	3.7763	2.2914	0.4364	0.7033	57.6167
	W	-6.1971	-1.6664	4.5306	6.1971	1.6664	3.9317	2.2653	0.4414	0.6772	59.7172
NO <sub>2</sub>	G	-6.4401	-2.2550	4.1851	6.4401	2.2550	4.3475	2.0925	0.4778	0.6337	53.4056
	W	-6.3672	-2.5023	3.8648	6.3671	2.5023	4.4347	1.9324	0.5174	0.6637	57.8910

The frontier molecular orbitals related to the reactivity of the dibenzo-18-crown-6 and its derivatives are reported in Table 1. Quantum parameters and corrosion inhibition efficiency were calculated using equations that can be seen in elsewhere [20-22]. The transition of electrons within



Molecules in the form of donations and acceptance occurs when HOMO and LUMO energy interact. HOMO energy indicates the tendency of molecules to donate electrons. Molecules that have electron donating groups have higher HOMO than those with electron withdrawing groups. The electron donating groups will donate electrons more intensely than electron withdrawing groups [24]. Table 1 shows that the HOMO energies for the DB18C6 and eleven substituted compound models follow the order of  $\text{NH}_2 > \text{OCH}_3 > \text{OH} > \text{CH}_3 > \text{CHCH}_2 > \text{H} > \text{F} > \text{COOCH}_3 > \text{COCH}_3 > \text{COOH} > \text{CHO} > \text{NO}_2$ . In general, this trend shows that the electronic donating groups within the framework of dibenzo-18-crown-6 ether increases the HOMO energies. Meanwhile, adding the electron-withdrawing groups on the dibenzo-18-crown-6 ether reduced the HOMO energies. Apparently, the  $\text{NH}_2$  substituent contributes to the highest HOMO energy and contrast, the  $\text{NO}_2$  substituent contributes to the lowest HOMO energy. This trend can be used as a preliminary prediction that crowns with  $\text{NH}_2$  substituent has the highest corrosion inhibitor efficiency.

The effect of substituents on the corrosion inhibitor performance is studied further by analyzing ionization energy. This energy describes the chemical reactivity of atoms and molecules. High reactivity is owned by atoms which have high ionization energy [25]. The energy trends ionization followed the HOMO energy trends as depicted on Table 1. The lowest  $\text{NH}_2$  electron ionization energy is derived from donation (5.093 eV). The highest ionization energy is produced by the  $\text{NO}_2$  electron withdrawing contribution (6.440 eV). These results indicate that  $\text{NH}_2$  enhances the reactivity of DB18C6, thus the  $\text{NH}_2$  substituted crown ether has a higher capability to bind to metal surfaces. The electronegativity values of substituted crown ethers can also be seen in Table 1. The DB18C6- $\text{NH}_2$  with a low electronegativity (2.341 eV) slowly reaches equalization and hence indicates a high inhibition efficiency. In contrast, DB18C6- $\text{NO}_2$  with a higher electronegativity (4.347 eV) and low reactivity which in turn indicates the low inhibition efficiency.



**Figure 2.** The calculated HOMO and LUMO energies, and electrostatic potential of the studied molecules determined using DFT method.

Figure 2 shows the frontier molecular orbital visualization ( $R = \text{NO}_2, \text{H}, \text{NH}_2$ ) calculated by B3LYP/6-31G(d) level of theory. It indicates that the HOMO of these crown ether compounds matches with the aromatic  $\pi$  system of the two benzene rings of DB18C6. The inductive effect of electron-donating substituent distributes the electron density on the aromatic  $\pi$  system and closer to a crown ether oxygen atom. The electron distribution in term of electrostatic potential (ESP) is also visualized in Figure 2. The ESP predicts the reactivity of the molecules according to electron distribution. It confirms the frontier molecular orbital visualization in which the inductive effect of electron-donating substituent enhances the electron density on the  $\pi$ -electron multiple bonds of benzene. In contrast, the electrostatic potential visualization from electron-withdrawing substituent leads to the opposite description. Apparently, it expected the enhancement of the  $\pi$ -electron in benzene contribution for interacting with metal surfaces.

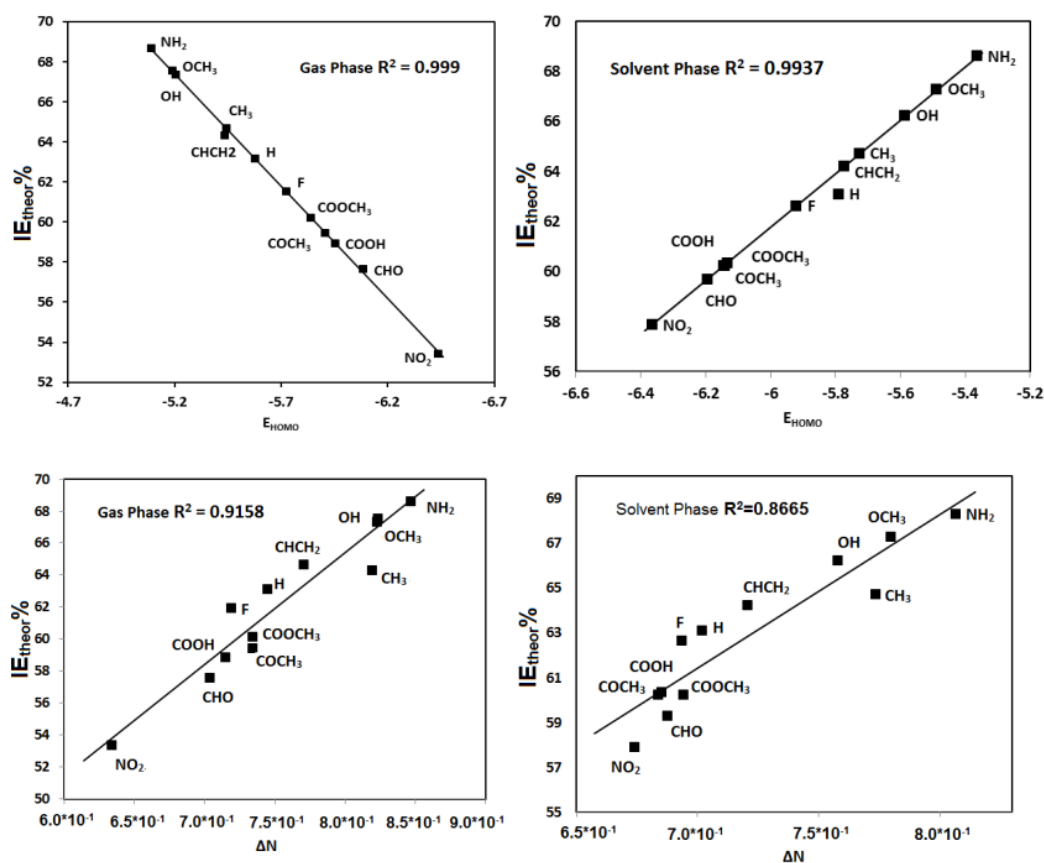


Figure 3. Correlation between  $E_{\text{HOMO}}$  and the number of electrons transferred ( $\Delta N$ ) with corrosion inhibition efficiency ( $IE\%$ ) of dibenzo-18-crown-6 derivatives in gas and solvent phase.

In order to study the correlation between other quantum chemical parameters and their corrosion inhibition performance, the inhibition efficiencies for dibenzo-18-crown-6 and eleven studied models have been determined as given formula [25]. The inhibition efficiency of dibenzo-18-crown-6 was 63.13 % [15]. The calculated inhibition efficiency values are depicted in Table 1. The corrosion inhibition efficiency data shows that the presence of electron donating substituents on the framework of DB18C6 increases inhibition efficiency by approximately 5.5 %, in going from  $\text{CHCH}_2$  to  $\text{NH}_2$

substituents. In contrast, the electron withdrawing substituents reduce the inhibition efficiency by 9.7 %, in going from F to NO<sub>2</sub> substituents. The highest inhibition efficiency is found with the electron donating substituent (NH<sub>2</sub>) and the lowest is produced using the electron withdrawing substituent (NO<sub>2</sub>). The correlation between the quantum chemical parameters and the corrosion inhibition efficiency is depicted in Figure 3. A good linear correlation has been identified between HOMO energies and inhibition efficiencies ( $r^2 = 0.9998$ ). Linear correlation also obtained from electrons transferred and inhibition efficiencies ( $r^2 = 0.9158$ ).

Table 1 shows the number of electrons transferred ( $\Delta N$ ). The magnitude of  $\Delta N$  values is closely related to the efficiency of corrosion inhibition and in accordance with previous studies from Lukovits [26]. The Lukovits study states that if  $\Delta N < 3.6$  then the inhibition efficiency increases. This is due to the increase in electron-donating abilities of inhibitors to donate electrons to the metal surfaces. Increased  $\Delta N$  values follow the order: NH<sub>2</sub> > OCH<sub>3</sub> > OH > CH<sub>3</sub> > CHCH<sub>2</sub> > H > F > COOCH<sub>3</sub> > COCH<sub>3</sub> > COOH > CHO > NO<sub>2</sub>. The result indicated that  $\Delta N$  values correlated strongly with the experimental and predicted inhibition efficiencies. The highest value of  $\Delta N$  is associated with the best inhibitor (NH<sub>2</sub> substituent), whereas the least  $\Delta N$  value is associated with the least inhibition efficiency (NO<sub>2</sub> substituent).

**Table 2.** Fukui and local softness indices for nucleophilic and electrophilic attacks in phenyl ring and oxygen ring of crown ether (R = NH<sub>2</sub> and NO<sub>2</sub>).

Atom	DB18C6-NH <sub>2</sub>				DB18C6-NO <sub>2</sub>			
	$f^+$	$f^-$	$\sigma^+$	$\sigma^-$	$f^+$	$f^-$	$\sigma^+$	$\sigma^-$
Phenyl ring					Phenyl ring			
C(3)	0.0349	0.0176	0.0127	0.0064	0.0211	0.0330	0.0076	0.0120
C(4)	0.0180	0.0237	0.0065	0.0086	0.0212	0.0112	0.0077	0.0040
C(35)	0.0181	0.0483	0.0065	0.0175	0.0220	0.0256	0.0079	0.0093
C(36)	0.0082	0.0086	0.0029	0.0031	0.0173	0.0009	0.0063	0.0003
C(37)	0.0292	0.0097	0.0106	0.0035	0.0279	0.0225	0.0101	0.0082
C(38)	0.0092	0.0492	0.0033	0.0179	0.0091	0.0029	0.0033	0.0010
Oxygen ring					Oxygen ring			
O(21)	0.0226	0.0082	0.0082	0.0030	0.0367	0.0072	0.0133	0.0026
O(22)	0.0162	0.0047	0.0058	0.0017	0.0276	0.0096	0.0100	0.0035
O(23)	-0.0070	-0.0097	-0.0025	-0.0035	0.0010	-0.0074	0.0003	-0.0027
O(24)	0.0157	0.0047	0.0057	0.0017	0.0276	0.0094	0.0100	0.0034
O(25)	0.0220	0.0082	0.0080	0.0030	0.0367	0.0072	0.0133	0.0026
O(26)	-0.0120	-0.0118	-0.0043	-0.0043	-0.0025	-0.0065	-0.0009	-0.0023

Table 2 shows the displays nucleophilic and electrophilic attacks in terms of Fukui and local softness indices in phenyl ring and oxygen ring of electron donating (NH<sub>2</sub>) and -withdrawing substituent (NO<sub>2</sub>). The phenyl ring ( $\pi$ -electron) and oxygen ring (donor heteroatom) of crown ethers were selected for local reactivity study due to the most possible binding sites to metal surface. For a nucleophilic attack on phenyl ring, the most reactive site of DB18C6-NH<sub>2</sub> is on the carbon atom number 3 (C3) and for electrophilic attack the most reactive site is the carbon atom number 38 (C38). In the DB18C6-NO<sub>2</sub> molecule the most reactive site for nucleophilic attack is in atom O(21)  $\approx$  O(25) and the favourable electrophilic attack is in atom C(3). The phenyl rings of DB18C6-NH<sub>2</sub> more capable to bind metal surfaces via  $\pi$ -electron than the phenyl rings of the DB18C6-NO<sub>2</sub> and other studied molecules in a nucleophilic reaction. It is confirmed by the maximum  $f^+$  and  $f^-$  values of DB18C6-NH<sub>2</sub> are the highest among the studied crown ether molecules.

#### 4. Conclusion



Quantum chemical parameters including the HOMO orbital energy ( $E_{\text{HOMO}}$ ) and the LUMO orbital energy ( $E_{\text{LUMO}}$ ), ionization potential (I), electron affinity (A), the absolute electronegativity ( $\chi$ ), hardness ( $\eta$ ), softness ( $\sigma$ ), the fraction of electron transferred ( $\Delta N$ ), and the inhibitors efficiencies dibenzo-18-crown-6 and its derivatives have been studied by B3LYP/6-31G(d) level of theory. To the system under consideration, the calculation results indicated that the highest occupied molecular orbital  $E_{\text{HOMO}}$  and the fraction of electron transferred ( $\Delta N$ ) have a good correlation with the corrosion inhibition efficiency (IE%). Electron donating substituents ( $\text{NH}_2$ ,  $-\text{OCH}_3$ ,  $-\text{OH}$ ,  $-\text{CH}_3$ ,  $-\text{CH}_2\text{CH}_3$ ) increases the inhibition efficiency, in contrast, electron withdrawing substituent  $-\text{COOCH}_3$ ,  $-\text{COOH}$ ,  $-\text{CHO}$ ,  $-\text{F}$ ,  $-\text{NO}_2$  have the opposite effect. It is found that  $\text{NH}_2$  substituent exhibits the highest inhibition efficiency, whereas  $\text{NO}_2$  substituent exhibits the lowest highest inhibition efficiency. The local reactivity from Fukui function confirmed that the pheny rings of crown ether have higher binding contribution to metal surfaces via delocalization of  $\pi$ -electron.

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