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Research Article

INHIBITORY POWER OF SOME ANTIRETROVIRAL DRUGS AGAINST COPPER CORROSION IN NITRIC ACID MEDIUM: THEORETICAL STUDY

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ABSTRACT

Density Functional Theory (DFT) method at B3LYP/6-31G (d) level has been used to study the inhibition properties of abacavir, zalcitabine and zidovudine in copper corrosion. The quantum chemical parameters such as highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}), energy gap (ΔE), dipole moment (μ), electronegativity (χ), hardness (η), softness (S), electrophylicity index (ω) were calculated and discussed. The local reactivity has been studied through the Fukui and dual descriptor in order to predict the possible sites of nucleophilic and electrophilic attacks. Theoretical calculations showed that these compounds have a good capacity to inhibit corrosion.

Keywords: Abacavir, Zalcitabine, Zidovudine, Density Functional Theory, Copper Corrosion

1. INTRODUCTION

The corrosion of metals and their alloys causes many consequences to industries [1], including the replacement of corroded parts, accidents and risks of pollution, etc. Copper is widely used in industry because of its many properties [2]. During its use, most industrial equipment made of copper or alloys are brought into contact with acid solutions that are very aggressive and cause them to dissolve [3, 4],because these acid solutions are used to perform several operations on copper [5, 6]. A lot of research [7, 8] has been directed towards the fight against corrosion to help manufacturers to safeguard their installations and equipment. Among these different methods we have the use of organic or inorganic corrosion inhibitors. These inhibitors are an effective means to fight against corrosion. Inorganic substances including phosphates, chromates, dichromates, silicates, bromates, arsenates, tungstates, molybdates, chlorides and their derivatives have long been used to combat the dissolution of metals. Unfortunately these compounds [9] are mostly carcinogenic and pollute the environment, which is why much research today is directed towards organic inhibitors, which are not very toxic and stable at high temperatures [10-12]. Depending on the literature [13-18], organic compounds that have heteroatoms (S, P, O, N) in their molecular structure can offer special active electrons or vacant orbitals capable of accepting or giving electrons. Today, in order to meet the requirements of the international organization on the preservation of the environment, several researches have been oriented towards natural plant extracts [19, 20] and therapeutic molecules [21, 22].

Quantum chemical calculation is usually used to study the correlations between the corrosion inhibition and molecular properties of the inhibitors. Many studies in the literature [23-25] show the correlations between the organic molecules chemical reactivity and their descriptor parameters.

In the other hand, the quantum chemistry methods (Hartree-Fock, Post Hartree-Fock, and DFT) give the possibility to guess a mechanism of interactions between the organic molecules and the metal surface. They led to molecular parameters such as the lowest unoccupied molecular orbital E_{LUMO}, the highest occupied molecular orbital (E_{HOMO}), the energy gap (ΔE), the dipole moment (μ), the total energy (E_T), etc.

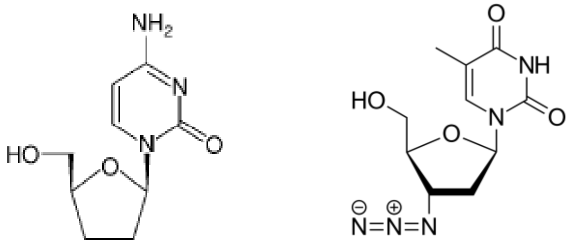
Density functional theory (DFT) [26-28] methods has become very popular in recent because it considered as a very useful method to probe the inhibitor/metal interaction as well as to analyze experimental data. It provides insights into thechemical reactivity and selectivity in terms of global parameters (electronegativity (χ), hardness(η), softness (S)) and local parameters such as Fukui function (f_k^+ or f_k^-) and dual descriptor $\Delta fk(r)$.

The power of the inhibition depends on the molecular structure of the inhibition. In the present study the objective is to correlate the structure of three antiretroviral molecules which are abacavir, zalcitabine and zidovudine with their inhibition efficiency against copper corrosion in nitric acid. In addition the use of these calculations can also predict the corrosion effectiveness of these related compounds, which would facilitate their practical use in corrosion control.

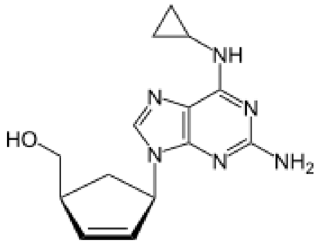
2. MATERIALS AND METHODS

2.1. Molecules structures

The chemical structures of the compounds studied are given in Figure 1.



(A- Zalcitabine) **(B- zidovudine)**



(C- Abacavir)

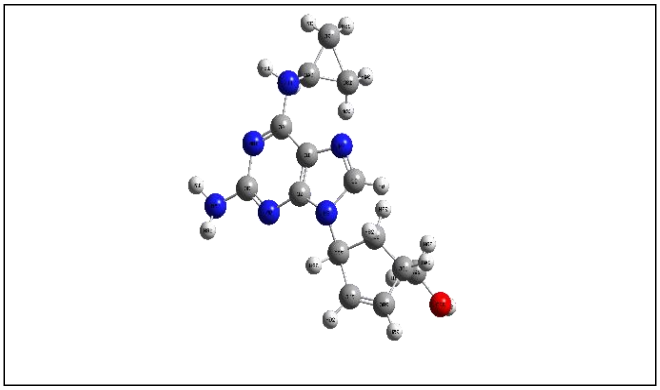
Fig. 1: Molecular structures of the investigated inhibitors

(A) *2′-3′-dideoxycytidine,* ***(B)*** *1-[(2R, 4S, 5S)-4-azido-5-(hydro- xylmethyl) oxolan-2-yl]-5-mehtyl-pyrimidine-2-4-dione,* ***(C)*** *[(1S, 4R)-4-[2amino-6-(cyclopropylamino) -9H-purin-9-yl] cyclopent-2-enyl]méthanole*

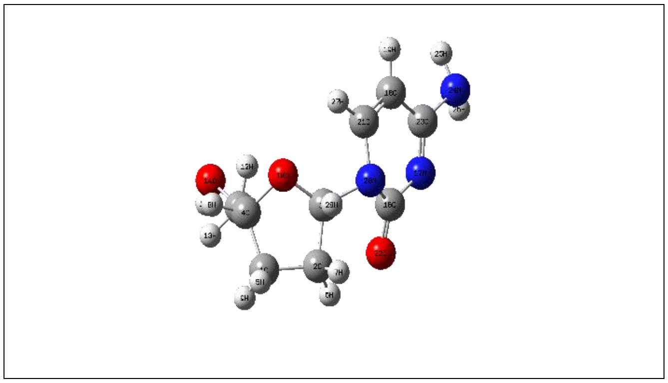
2.2. Quantum chemical calculations

In this work all calculations were done by GAUSSIAN 09W software [29]. The molecules structure was geometrically optimized, using DFT at B3LYP level [30-32] with 6-31 G (d) basis set [33].

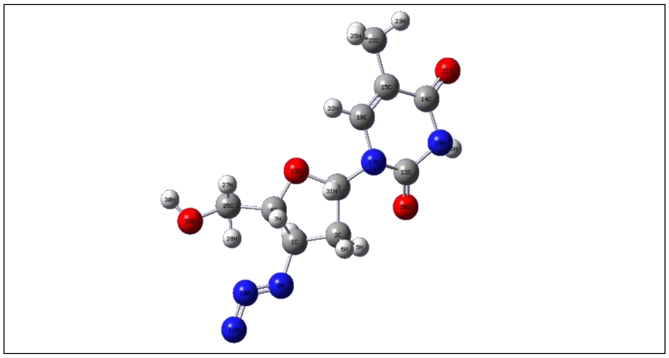
DFT used in this work has become a popular method today, it provides results comparable to other methods (Hatree-Fock method and post-Hatree-Fock methods). The electronic correlation is included in the DFT, so the results are better for accessible calculation times. It gives access to the descriptor parameters of each molecule which allow to predict the inhibition properties of the molecules. The optimized molecular structures of the molecules studied, obtained by use of the hybrid DFT functional (B3LYP/6-31G (d)) are shown in Figure 2.



Abacavir (ABA)



Zalcitabine (ZAL)



Zidovudine (ZID)

Fig. 2: Optimized structures of ABA, ZAL and ZID with B3LYP/6-31G (d) method

3. RESULTS AND DISCUSSION

3.1. Global reactivity

The values of the calculated quantum chemical global parameters are listed in table 1. E_{HOMO} [34] is often associated with the electron donating ability of a molecule. An increase in the values of E_{HOMO} can facilitate the adsorption and therefore the inhibition efficiency, by indicating the disposition of the molecule to donate electrons to an appropriate acceptor with empty molecular orbital. The LUMO energy on the other hand [34], indicates the ability of the molecule to accept electrons.

Table 1: Quantum chemical parameters of the studied compounds calculated using B3LYP/6-31G(d)

Parameters	ABA	ZAL	ZID
E_{HOMO} (eV)	-5.048864	-5.948096	-6.210304
E_{LUMO} (eV)	-0.68816	-0.979859	-1.18864
Energy gap ΔE (eV)	4.360704	4.968237	5.021664
Dipole moment μ (D)	2.8609	6.7915	4.7934
Ionization energy I (eV)	5.048864	5.948096	6.210304
Electron affinity A (eV)	0.68816	0.979859	1.18864
Electronegativity χ (eV)	2.868512	3.4639775	3.699472
Hardness η (eV)	2.180352	2.48411185	2.510832
Softness σ $(eV)^{-1}$	0.458641	0.402558	0.398274
Fraction of electron transferred ΔN	0.483945	0.306451	0.256972
Electrophylicity indexω	1.913189	2.415171	2.725409
Total energy E_T(Ha)	-947.169	-950.598	-963.469

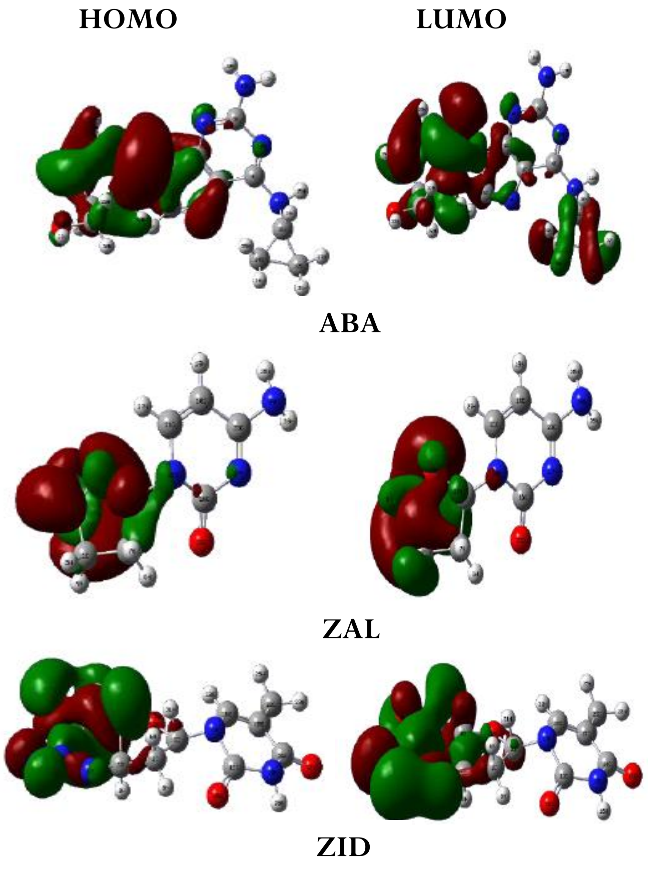


Fig. 3: HOMO-LUMO diagrams of the molecules

The energy of the highest occupied molecular orbital (E_{HOMO}) values of the three molecules consigned above in the table are lofty. These values reveal their capacity to give some electrons to a suitable acceptor endowed with an orbital vacant of low energy. The E_{HOMO} values of the molecules studied increase in the following order: ABA > ZAL > ZID, which means that ABA could have high inhibition efficiency.

These molecules do not only supply electrons to the «d» orbitals of metal ions such as Cu^{2+}([Ar] $3d^9$), but they can also receive electrons from these «d» orbitals, leading to a mutual exchange of electrons. In our case, the low E_{LUMO} values show that these molecules tend to receive electrons.

The lower the values of E_{LUMO}, the more probable it is that the molecules accept electrons. The binding capacity of the inhibitor to the metal surface increases with increasing HOMO and decreasing LUMO energy values because the geometry of the inhibitor's base state and the nature of its frontier molecular orbitals, HOMO and LUMO, are involved in the inhibition process. It should be noted that the electron density of the HOMO location in each molecule is mainly distributed near the nitrogen (N) and oxygen (O) atoms showing that these are the preferred sites for adsorption, whereas the LUMO density was distributed almost of the entire molecules. The HOMO-LUMO diagrams of the molecules are shown in Figure 3.

In the same way, low values of the energy gap $\Delta E = E_{LUMO} - E_{HOMO}$ lead to good inhibition efficiencies because [35] the energy to remove an electron from the last occupied orbital will be low. In this study the lower values of the energy gap when compared with that of many molecules in the literature confirms the good capacity of the molecules to inhibit copper corrosion. Comparing the different values of ΔE in table 1, ABA has the lowest value therefore it could be the good inhibitor.

The dipole moment is another parameter of the electron distribution in a molecule and is the measure of the polarity of a polar covalent bond. High values of the dipole moment μ [36] will favor the accumulation of the inhibitor molecules on the metallic surface. However, several authors [37, 38] state that the inhibition efficiency increases with increasing values of dipole moment. So in general [39], there is no significant relationship between the dipole moment values and inhibition efficiency.

According to Koopman's theorem [40], the energies of the HOMO and LUMO orbitals of the inhibitor molecule are related to the ionization potential *I*, and the electron affinity, *A*, respectively, by the following relationships:

$$\mathrm{I} = -\mathrm{E}_{\mathrm{HOMO}} \quad (1)$$

$$\mathrm{A} = -\mathrm{E}_{\mathrm{LUMO}} \quad (2)$$

Ionization energy is a fundamental descriptor of the chemical reactivity of atoms and molecules. High ionization energy [41] indicates high stability and chemical inertness and small ionization leads to high reactivity of atoms and molecules. The low values of ionization energy (5.048, 5.948 and 6.210 eV) respectively of abacavir, zalcitabine and zidovudine will certainly be one of the causes of their high inhibition efficiencies.

Electronegativity (χ), absolute hardness (η) and softness (σ) are important properties to measure the molecular stability and reactivity. These reactivity parameters have been respectively deduced from the following relationships:

$$\chi = \frac{I+A}{2} \quad (3)$$

$$\eta = \frac{\mathrm{I}-\mathrm{A}}{2} \quad (4)$$

$$\sigma = \frac{1}{\eta} \quad (5)$$

When two systems, metal and inhibitor, are brought together, electrons will flow from lower χ (inhibitor) to higher χ (metal), until the chemical potentials become equal [42]. In our case, the electronegativity values of the three molecules are lower than copper (4.98), so it's possible the electrons could be moving from the molecules to the copper. The chemical hardness represents the resistance towards the deformation or polarization of the electron cloud of the atoms, ions or molecules under small perturbation or chemical reaction. A good inhibitor has a high softness value and a low hardness value [43]. In our work, the low hardness values of the molecules (2.1803eV, 2.4841eV and 2.5108eV) compared with many other compounds, will be the good performance as a corrosion inhibitor of copper in the studied medium. It is evident that in that case the softness values are high since softness is the inverse of hardness.

The global electrophilicity index (ω), introduced by Parr as a measure of energy lowering [44] due to maximal electron flow between donor and acceptor is given by:

$$\omega = \frac{\mu_p^2}{2\eta} \quad (6)$$

That parameter measures the propensity of chemical species to accept electrons. A high value of ω describes a good electrophile while a small value describes a good nucleophile [45]. In this work the obtained values (1.9131eV, 2.4151eV and 2.7254eV) shows the good capacity of the three (3) molecules studied to accept electrons.

This reactivity index measures the stabilization in energy when the system acquired an additional electronic charge ΔN from the environment. Thus the fraction ΔN of electrons transferred from the inhibitor to the metallic surface [42] is given by:

$$\Delta N = \frac{\chi_{Cu} - \chi_{inh}}{2(\eta_{Cu} + \eta_{inh})} \quad (7)$$

Where χ_{Cu}, η_{Cu}, χ_{inh} and $\eta_{inh}$are respectively the absolute electronegativity and hardness of copper and the inhibitor. We use the theoretical value of $\chi_{Cu} = 4.98$ eV/mol[42]and $\eta_{Cu} = 0$ [42] for the calculation of the number of electrons transferred.The Fraction of electron transferred (ΔN)of the molecules are recorded in the table 1. According to Lukovits's study [46], the positive sign of this value is an indicator of the tendency of a molecule to donate electrons to the metal, this that means the inhibition efficiency increases by increasing electron donating ability of the inhibitors to the metal surface. In this work, the fractions of electrons transferred from molecules are positive and they are in the order ABA > ZAL >ZID so, they can be good inhibitors.ABA could be the best inhibitor.

The total energy (E_T) calculated by quantum chemical method is also a beneficial parameter. For the three molecules $E_T < 0)$ and $\eta > 0$, the charge transfer from each molecule to the metal is energetically favorable [47].

3.2. Local reactivity

The local reactivity of the studied molecules can be analyzed through the condensed Fukui indices. The condensed Fukui functions indicate the atoms in a molecule that have a tendency to either donate (nucleophile character) or accept (electrophile character) an electron or pair of electrons. The nucleophilic and electrophilic functions for an atom k [48] can be computed using the finite difference approximation as follows:

$$f_k{}^+=[q_k(\mathrm{N+1})-q_k(\mathrm{N})] \text{ for nucleophilic attack} \qquad (8)$$

$$f_k{}^-=[q_k(\mathrm{N})-q_k(\mathrm{N-1})] \text{ for electrophilic attack} \qquad (9)$$

Where $q_k(\mathrm{N}+1)$, $q_k(\mathrm{N})$ and $q_k(\mathrm{N}-1)$ are defined as Mulliken charge of the anionic, neutral and cationic species respectively.

Another descriptor known as dual descriptor [49] and defined as the difference between the nucleophilic and electrophilic Fukui functions has been recently used:

$$\Delta f_k(\mathrm{r})=f_k^+(\mathrm{r})-f_k^-(\mathrm{r}) \qquad (10)$$

If $\Delta f_k(\mathrm{r}) > 0$, then the site is favoured for a nucleophilic attacks, whereas if $\Delta f_k(\mathrm{r}) < 0$, then the site may be favoured for an electrophilic attack. The different values are recorded in Tables 2-4.

Table 2: Fukui indices and dual descriptors for the atoms of ABA calculated using Mullikencharges.

Atoms	q_k(N + 1)	q_k(N)	q_k(N - 1)	f_k^+	f_k^-	Δf_k(r)
1 C	-0.001857	0.188592	0.010598	-0.190449	0.177994	-0.368443
2 C	0.006307	0.456228	0.011146	-0.449921	0.445082	-0.895003
3 C	0.001755	0.531119	0.002192	-0.529364	**0.528927**	**-1.058291**
4 C	0.002299	0.37704	-0.00074	-0.374741	0.37778	-0.752521
5 C	-0.039466	0.228068	0.020644	-0.267534	0.207424	-0.474958
6 H	0.001993	0.193876	0.003053	-0.191883	0.190823	-0.382706
7 N	0.061336	-0.506832	-0.007981	0.568168	-0.498851	1.067019
8 N	0.07863	-0.52661	0.07744	0.60524	-0.60405	1.20929
9 N	-0.000892	-0.523238	0.000045	0.522346	-0.523283	1.045629
10 N	-0.003265	-0.525401	-0.00237	0.522136	-0.523031	1.045167
11 N	0.000859	-0.542826	0.000629	0.543685	-0.543455	1.08714
12 C	0.079971	-0.32551	0.232161	0.405481	-0.557671	0.963152
13 C	0.203947	-0.296317	0.224471	0.500264	-0.520788	**1.021052**
14 C	-0,033097	-0,025134	-0,017968	-0,007963	-0,007166	-0.000797
15 H	-0.00047	0.320127	-0.003115	-0.320597	0.323242	-0.643839
16 N	0.001255	-0.726933	-0.000009	**0.728188**	-0.726924	**1.455112**
17 H	-0.00003	0.332385	-0.000016	-0.332415	0.332401	-0.664816
18 H	-0.000022	0.334952	-0.000053	-0.334974	0.335005	-0.669979
19 C	-0.007461	-0.175941	-0.012751	0.16848	-0.16319	0.33167
20 C	0.160368	-0.061201	0.082374	0.221569	-0.143575	0.365144
21 C	-0.066325	-0.174511	0.142305	0.108186	-0.316816	0.425002
22 C	0.548637	-0.126706	-0.023566	0.675343	-0.10314	0.778483
23 C	-0.027183	-0.377472	0.148713	0.350289	-0.526185	0.876474
24 H	0.000823	0.148443	0.005606	-0.14762	0.142837	-0.290457
25 H	-0.003931	0.154518	0.000445	-0.158449	0.154073	-0.312522
26 H	0.004537	0.143975	0.004096	-0.139438	0.139879	-0.279317

Continued…

Atoms	q_k(N + 1)	q_k(N)	q_k(N - 1)	f_k^+	f_k^-	Δf_k(r)
27 H	0.000071	0.207608	0.004712	-0.207537	0.202896	-0.410433
28 H	0.01807	0.220799	0.00157	-0.202729	0.219229	-0.421958
29 C	0.013625	-0.013376	0.011881	0.027001	-0.025257	0.052258
30 H	-0.000252	0.122277	-0.00065	-0.122529	0.122927	-0.245456
31 H	-0.001573	0.159097	-0.000655	-0.16067	0.159752	-0.320422
32 O	0.005501	-0.63748	0.000043	0.642981	-0.637523	1.280504
33 H	-0.000184	0.396375	-0.000023	-0.396559	0.396398	-0.792957
34 H	-0.012621	0.211891	-0.002054	-0.224512	0.213945	-0.438457
35 H	0.016655	0.103125	-0.032123	-0.08647	0.135248	-0.221718
36 H	-0.008292	0.209692	-0.001251	-0.217984	0.210943	-0.428927
37 H	0.020521	0.09285	-0.033168	-0.072329	0.126018	-0.198347
38 H	-0.000404	0.159411	-0.004648	-0.159815	0.164059	-0.323874
39 H	-0.019837	0.273041	0.159018	-0.292878	0.114023	-0.406901

Table 3: Fukui indices and dual descriptors for the atoms of ZAL calculated using Mullikencharges

Atoms	q_k(N + 1)	q_k(N)	q_k(N - 1)	f_k^+	f_k^-	Δf_k(r)
1 C	0.011065	-0.274147	0.011065	0.285212	-0.285212	0.570424
2 C	0.007859	-0.301621	0.007859	0.30948	-0.30948	0.61896
3 C	0.004973	0.266808	0.004973	-0.261835	0.261835	-0.52367
4 C	-0.037189	0.038486	-0.037189	-0.075675	0.075675	-0.15135
5 H	-0.001571	0.166105	-0.001571	-0.167676	0.167676	-0.335352
6 H	0.00663	0.208949	0.00663	-0.202319	0.202319	-0.404638
7 H	0.000114	0.158911	0.000114	-0.158797	0.158797	-0.317594
8 H	0.025575	0.140066	0.025575	-0.114491	0.114491	-0.228982
9 H	-0.003571	0.157264	-0.003571	-0.160835	0.160835	-0.32167
10 O	0.053994	-0.512891	0.053994	0.566885	-0.566885	1.13377
11 C	0.773925	-0.210642	0.773925	**0.984567**	-0.984567	**1.969134**
12 H	-0.051681	0.265749	-0.051681	-0.31743	0.31743	-0.63486
13 H	-0.048128	0.192208	-0.048128	-0.240336	0.240336	-0.480672
14 O	0.089184	-0.645243	0.089184	0.734427	-0.734427	1.468854
15 H	-0.003733	0.40615	-0.003733	-0.409883	0.409883	-0.819766
16 C	-0.004869	0.68155	-0.004869	-0.686419	**0.686419**	**-1.372838**
17 N	0.037001	-0.511151	0.037001	0.548152	-0.548152	1.096304
18 C	0.04974	-0.199099	0.04974	0.248839	-0.248839	0.497678
19 H	-0.002253	0.140004	-0.002253	-0.142257	0.142257	-0.284514
20 N	0.040144	-0.507151	0.040144	0.547295	-0.547295	1.09459
21 C	-0.019781	0.058753	-0.019781	-0.078534	0.078534	-0.157068
22 O	0.022877	-0.484288	0.022877	0.507165	-0.507165	1.01433
23 C	-0.011531	0.444931	-0.011531	-0.456462	0.456462	-0.912924
24 N	-0.000593	-0.726753	-0.000593	0.72616	-0.72616	1.45232
25 H	0.000037	0.323437	0.000037	-0.3234	0.3234	-0.6468
26 H	0.000133	0.339515	0.000133	-0.339382	0.339382	-0.678764
27 H	0.001625	0.193691	0.001625	-0.192066	0.192066	-0.384132
28 H	0.060025	0.190411	0.060025	-0.130386	0.130386	-0.260772

Table 4: Fukui indices and dual descriptors for the atoms of ZID calculated using Mulliken charges

Atoms	q_k(N + 1)	q_k(N)	q_k(N - 1)	f_k^+	f_k^-	Δf_k(r)
1 C	0.004949	0.001833	0.034891	0.003116	-0.033058	0.036174
2 C	-0.005347	-0.322875	-0.311675	0.317528	-0.0112	0.328728
3 C	-0.008138	0.298133	0.286433	-0.306271	0.0117	-0.317971
4 C	0.038489	0.025907	0.057827	0.012582	-0.03192	0.044502
5 H	-0.00911	0,222588	0,18049	-0,231698	0,042098	-0,273796
6 H	-0.00215	0.174231	0.139824	-0.176381	0.034407	-0.210788
7 H	0.036613	0.148305	0.102898	-0.111692	0.045407	-0.157099
8 H	-0.000239	0.18198	0.117653	-0.182219	0.064327	-0.246546
9 N	-0.261547	-0.244281	-0.360672	-0.017266	0.116391	-0.133657
10 N	-0.172291	0.047796	-0.01566	-0.220087	0.063456	-0.283543
11 N	0.495106	-0.111581	-0.353793	0.606687	**0.242212**	**0.364475**
12 O	-0.034937	-0.536798	-0.564833	0.501861	0.028035	0.473826
13 C	0.007439	0.688554	0.676641	-0.681115	0.011913	**-0.693028**
14 C	0.013922	0.504944	0.499009	-0.491022	0.005935	-0.496957
15 C	-0.049173	0.072231	0.062236	-0.121404	0.009995	-0.131399
16 H	0.000236	0.365582	0.350488	-0.365346	0.015094	-0.38044
17 N	-0.063686	-0.513957	-0.518179	0.450271	0.004222	0.446049
18 C	0.007191	-0.017007	-0.003986	0.024198	-0.013021	0.037219
19 N	-0.002182	-0.599511	-0.610577	0.597329	0.011066	0.586263
20 O	-0.023365	-0.476987	-0.473004	0.453622	-0.003983	0.457605
21 O	-0.026521	-0.482249	-0.514445	0.455728	0.032196	0.423532
22 C	0.001958	-0.508204	-0.506431	0.510162	-0.001773	0.511935
23 H	-0.001063	0.19465	0.175787	-0.195713	0.018863	-0.214576
24 H	-0.00281	0.182135	0.171706	-0.184945	0.010429	-0.195374
25 H	-0.000544	0.162678	0.154067	-0.163222	0.008611	-0.171833
26 C	0.811218	-0.145565	-0.166646	**0.956783**	0.021081	**0.935702**
27 H	0.026151	0.221758	0.074144	-0.195607	0.147614	-0.343221
28 H	0.039534	0.24668	0.204563	-0.207146	0.042117	-0.249263
29 O	0.19447	-0.596857	-0.60264	0.791327	0.005783	0.785544
30 H	0.005399	0.420488	0.3338	-0.415089	0.086688	-0.501777
31 H	-0.019155	0.196742	0.180149	-0.215897	0.016593	-0.23249
32 H	0.198895	0.198656	0.199932	0.000239	-0.001276	0.001515

From the tables, one can see that many atoms with high negative charge densities could be active adsorption centers; they could have strongest ability to bond the metal surface.

f_k^+ measures changes of density when the molecule gains electrons and it corresponds to reactivity with respect to nucleophilic attack, whereas f_k^- corresponds to reactivity with respect to electrophilic attack or when the molecule loses electrons.

In table 2, the preferred site for nucleophile attacks is around N(16) atom, f_k^+ and Δf_k(r) are maximum what is confirmed by the lack of electron cloud around the nitrogen atom while the preferred site for electrophile attacks is near C (3) where f_k^- the maximum value and Δf_k(r) $<$ 0 of abacavir molecule. For zalcitabine, the values are recorded in table 3, these values reveal that, C (11) atom is the probable site for nucleophilic attack because it has the highest value of f_k^+ and Δf_k(r) .On the other hand, C (16) atom is the probable site for electrophilic attack with maximum negative value of f_k^- and Δf_k(r)$<$0. In table 4, we can observed that C(26) in the LUMO region, with maximum value of f_k^+ and (Δf_k(r)$>$ 0) is the probable site for nucleophilic attack, whereas N (11) having the highest value of f_k^-, but does not have the negative value of $(\Delta f_k(r) < 0)$. Therefore C (13) in the HOMO region which has $(\Delta f_k(r) < 0)$ is the probable site for electrophilic attack of zidovudine molecule.

4. CONCLUSION

The results of this study can be concluded as follows:

- Abacavir, zalcitabin and zidovudine can be used as copper corrosion inhibitors in acid environments.
- The calculations show that the compound abacavir has the highest HOMO level and the lowest LUMO level compared to obtained parameters for zalcitabine and zidovudine. This can explain that the highest inhibition efficiency of abacavir is due to the increasing HOMO energy and the decreasing LUMO energy and energy gap (ΔE).
- Fukui function and dual descriptor show the nucleophilic and electrophilic attacking sites in the investigated inhibitors.

5. REFERENCES

1. Hoar T P, Hurlen T. *Proc. 8th Meeting CITCE,* 1956; 45.
2. Nunéz L, Reguera E, Corvo F, Gonzalez C. Corros. Sci., 2005; **2(47):**461-484
3. Ho CE, Chen WT, Kao CR. *J. Electron. Mater.* 2001; **30**:379-385.
4. Breslin CB, Macdonald DD. *Por. Electro. Acta*, 1998; **4(44):**643-651.
5. Qiang Y, Zhang S, Guo L, Zheng X, Xiang B, Chen S. *Cor. Sci.*, 2017; **119**:68-78.
6. *Olasunkanmi LO, Obot IB, Kabanda MM, Ebenso EE. J. Phys. Chem. C,* 2015; **28(119):**16004-16019.
7. Niamien PM, Essy FK, Trokourey A, Yapi A, Aka HK, Diabate D. *Mat. Chem. Phys.*, 2012; **1(136):**59-65
8. Obot I B, Obi-Egbedi N O. *Cor. Sci.*, 2010; **1(52):**198-204.
9. Sharmila A, Prema AA, Salayaraj PA. *J. Chem.*, 2010; 3(1):74-81
10. Lowmunkhong P, Ungthararak D, Sutthivaiyakit P. *Cor. Sci.* 2010; **1(52):**30-36.
11. Singh AK, Quraishi MA. *Cor. Sci.,* 2010 ; **1(52):**152-160.
12. Chauhan LR, Gunasekaran G. *Cor. Sci.*, 2007 ; **3(49):**1143-1161.
13. El Adnani Z, Mcharfi M, Sfaira M, Benzakour M et al. *Cor. Sci.*, 2013; **68(1):**223-230.
14. Popova A, Christov M, Zwetanova A. *Cor. Sci.,* 2007; **5(49):**2131-2143.
15. Chafiq M, Chaouiki A, Lgaz, H. et al. *Res. Chem. Intermed*. 2020; **6(46):**2881-2918
16. Mohanapriya N, Kumaravel M, Lalithamani B. *J. Electrochem. Sci. Technol*. 2020; **11(2):**117-131
17. Chidiebere MA, Oguzie EE, Liu L. *Mat. Chem. Phys.*, 2015; **156(1):**95-104.
18. Ebenso EE, Isabirye DA, Eddy NO. *Int. J. Mol. Sci.* 2010; **11(6):**2473-2498.
19. Dehghani A, Bahlakeh G, Ramezanzadeh B, Ramezanzadeh M. *J. Mol. Liq.,*2019;**279:**603-624.
20. Prasad D, Haldha R, Singh G, Kumar A. *J. Mol. Liq*. 2018; **258**:89-97.
21. Tigori MA, Bony FN, Niamien PM, Yapo AJ, Trokourey A. *Ar. Appl. Sci. Re.,* 2016, **8(5):**18-32.
22. Ouattara S, Tigori MA, Kouakou V et al. *J. Chem. Bio. Phy. Sci*., 2019; **9(4):**253-273.
23. Wazzan NA, Mahgoub FM. *Open J. Phys. Chem*., 2014; **4(1):**6-14.
24. Eddy NO, Momoh-Yahaya H, Oguzie EE. *J. Adv. Res.*, 2015; **6(2):**203-217.
25. 25. Ju H, Kai ZP, Li Y. *Cor. Sci*., 2008; **50(3):**865-871.
26. Kandemirli F, Sagdinc S. *Cor. Sci*. 2007; **49(5):**2118-2130.
27. 27. Garnet Kin-Lic Chan, fresh A. *J Chem. Phys.* 1999; **110**:4710-4723.
28. Obot IB, Obi-Egbedi NO, *Current Appl. Phys*. 2011; **11(3):**382-392.
29. Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR et al. *Gaussian 09,* 2009.
30. Becke AD, *J. Chem. Phys*. 1993; **98**:1372-1377.
31. Lee C, Yang W, Parr RG, *Phys. Rev. B*. 1988; **37**:785-789.
32. Yang W, Parr RG. *Proc. Natl. Acad. Sci*.1985; **82(20):**6723-6726.
33. Zhang SG, Lei W, Xia MZ, Wang FY. *J. of Molec. Stru (Theochem).* 2005; **732(1-3):**173-182.
34. Bentiss F, Bouanis M, Mernari B, Traisnel M, Vezin H, Lagrenee M. *Appl. Surf. Sci*. 2007; **253**(7):3696-3704
35. Awad MK, Mustafa MR, Abo Elnga MM. *J Mol Struct (Theochem*), 2010, **959(1-3):**66-74
36. Parr RG, Donelly RA, Levy M, Palke WE. *J. Chem. Phys.* 1978; **68(8):**3801-3807.

37. Quraishi MA, Sardar R. *J. Appl. Electrochem*. 2003; **33**:1163-1168.
38. Khaled K F, Babic-Samardzija K, Hackerman N. *Electro. Acta* 2005; **50(12):**2515-2520.
39. Bereket G, Hür E, Oretir C, *J. Mol. Struc. THEOCHEM* 2002; **578(1-3**):79-88.
40. Koopmans T. *Physica,* 1934; **1(1-6):**104-113.
41. Gece G, *Cor. Sci*. 2008; **50(11):**2981-2992
42. Pearson RG, *Inorg. Chem*. 1988; **27(4):**734-740.
43. Obot IO, Gasem ZM. *Corros. Sci.,* 2014, **83:**359-366.
44. Parr RG, Szentpaly L, Liu S. *J. Am. Chem. Soc.*, 1999; **121(9):**1922-1924
45. Khattabi M, Benhiba F, Tabti S. et al. *J. Mol. Struct.*, 2019; **1196**:231-244
46. Lukovits I, Kalman EF. *Corrosion,* 2001; **57(1):**3-8. .
47. Hegazy MA, Atlam FM. *J. Mol. Liq*. 2016; **218**:649-662.
48. Yang W, Mortier WJ. *J. Am. Chem. Soc.*, 1986; **108(19):**5708-5711.
49. Morell C, Grand A, Toro-Labbé A. *Chem. Phys. Lett*. 2006; **425(4-6):**342.