Adsorption and inhibitive properties of a new synthesized guanidine derivative on corrosion of copper in 0.5 M H₂SO₄

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1. Introduction

Due to its excellent thermal conductivity and good mechanical workability, copper is a material commonly used in heating and cooling systems. Scale and corrosion products have a negative effect on heat transfer, and they cause a decrease in heating efficiency of the equipment, which is why periodic descaling and cleaning in sulphuric acid pickling solutions are necessary. The use of copper corrosion inhibitors in such conditions is necessary since no protective passive layer can be expected. The possibility of the copper corrosion prevention has attracted many researchers so until now numerous possible inhibitors have been investigated. Amongst them there are inorganic inhibitors [1], but in much greater numbers there are organic compounds and their derivatives such as azoles [2–5], amines [6,7], amino acids [8] and many others. It is noticed that, the presence of heteroatoms such as nitrogen, sulphur, phosphorous in the organic compound molecule improves its action as copper corrosion inhibitor. This is explained by the presence of vacant d orbitals in copper ions that form coordinative bonds with atoms able to donate electrons. Interaction with rings containing conjugated bonds, π-electrons, is also present [9].

It is known that the mechanism of copper electrodeposition/dissolution strongly depends on the medium. Extensive research on the mechanism of the anodic dissolution of copper in sulphate solutions has been performed and a number of different dissolution mechanisms have been proposed. There is a general agreement in the literature that the process of Cu dissolution/deposition goes through Cu⁺ ions, adsorbed Cu(I) species or intermediate Cu⁺ compounds [10–16] as follows:

$$\text{Cu} - \text{e}^- \rightarrow \text{Cu}^{+}$$  \hspace{1cm} (1)

$$\text{Cu}^{+} + \text{e}^- \rightarrow \text{Cu}^{2+}$$  \hspace{1cm} (2)

It was concluded that the first step was much faster than the second one in sulphate solutions.

In continuation of the work on acid corrosion inhibitors [17–20], a new synthesized and safe corrosion inhibitor namely N-(5,6-diphenyl-4,5-dihydro-[1,2,4]triazin-3-yl)-guanidine (NTG) has been studied on copper in 0.5 M H₂SO₄; several chemical and electrochemical techniques have been used to investigate the effect of NTG on corrosion inhibition of copper. The quantum chemistry and the molecular dynamics simulation methods were used to elucidate the adsorption behaviour of NTG at copper surface in water. Correlation between the inhibition efficiency and the structural properties of NTG is suggested.

2. Experimental details

Fig. 1 shows the chemical structure of NTG which obtained by refluxing guanidine hydrochloride with 5,6-diphenyl-4,5-dihydro-[1,2,4] triazine-3-thiol in DMF for 2 h according to the following reaction:
1H NMR and FT-IR spectroscopies as well as the melting point of NTG are shown in Table 1.

The weight loss experiments were carried out using rectangular copper coupons and their chemical composition was given in Table 2. These coupons have dimensions of length 3.0 cm, width 1.0 cm, and thickness 0.20 cm with an exposed total area of 7.6 cm². A copper rod of the same composition was mounted in Teflon with an exposed area of 0.4 cm² and used for polarization and impedance measurements. The coupons were polished, dried and weighted, and then suspended in 200-ml aerated solution of 0.5 M H₂SO₄ without and with different concentrations of NTG for an exposure period of 24 h. After the designated exposure to the test solution, the specimens were rinsed with distilled water, washed with acetone to remove a film possibly formed due to the inhibitor, dried between two tissue papers, and weighted again. Weight loss measurements were made in triplicate and the loss of weight was calculated by taking an average of these values.

Electrochemical experiments carried out using copper specimens mounted in Teflon. An epoxy resin was used to fill the space between Teflon and copper electrode. The electrochemical measurements were performed in a typical three-compartment glass cell consisting of the copper specimen as a working electrode (WE), platinum mesh as a counter electrode (CE), and a saturated calomel electrode (SCE) as the reference electrode. The counter electrode was separated from the working electrode compartment by fritted glass. The reference electrode was connected to a Luggin capillary to minimize IR drop. Solutions were prepared from bidistilled water of resistivity 13 MΩ cm. Prior to each experiment, the specimen was polished with a series of emery papers of different grit sizes up to 4/0 grit size, polished with Al₂O₃ (0.5 mm particle size), washed several times with bidistilled water then with acetone and dried using a stream of air. The electrode potential was allowed to stabilize 60 min before starting the measurements. The aggressive environment used was 0.5 M H₂SO₄ solution with different concentrations of NTG. All experiments were conducted at 303 K and kept constant using water thermostat.

Potentiodynamic polarization curves were obtained by changing the electrode potential automatically from −850 up to +1100 mV SCE with a scan rate of 1.0 mV s⁻¹.

EIS measurements were carried out at a frequency range of 100 kHz to 50 mHz with an amplitude of 5 mV peak-to-peak using ac signals at open circuit potential.

Measurements were performed with a Gamry Instrument Potentiostat/Galvanostat/ZRA. This includes a Gamry Framework system based on the ESA400, Gamry applications that include DC105 for dc corrosion measurements, EIS300 for electrochemical impedance spectroscopy measurements along with a computer for collecting data. A BRUKE DPX-300 nuclear magnetic resonance spectroscopy was used to determine the structure of NTG. The chemical structure of the commercial copper electrode is given in Table 2.

### Table 1

<table>
<thead>
<tr>
<th>NTG concentration/M</th>
<th>Corrosion rate/mg m⁻² h⁻¹</th>
<th>Inhibition efficiency, ξ [%]</th>
<th>Surface coverage, θ [%]</th>
</tr>
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<tbody>
<tr>
<td>0</td>
<td>325.2</td>
<td>0.00</td>
<td>–</td>
</tr>
<tr>
<td>10⁻⁴</td>
<td>178.8</td>
<td>45.02</td>
<td>0.45</td>
</tr>
<tr>
<td>5 × 10⁻⁴</td>
<td>152.8</td>
<td>53.02</td>
<td>0.53</td>
</tr>
<tr>
<td>10⁻³</td>
<td>71.54</td>
<td>78.00</td>
<td>0.78</td>
</tr>
<tr>
<td>5 × 10⁻³</td>
<td>42.27</td>
<td>87.00</td>
<td>0.87</td>
</tr>
<tr>
<td>10⁻²</td>
<td>9.756</td>
<td>97.00</td>
<td>0.97</td>
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</table>

### Table 2

Chemical structure for the commercial copper electrode

<table>
<thead>
<tr>
<th>Element</th>
<th>Concentration (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>97.57</td>
</tr>
<tr>
<td>Zn</td>
<td>2.332</td>
</tr>
<tr>
<td>Ni</td>
<td>0.0109</td>
</tr>
<tr>
<td>Fe</td>
<td>0.0327</td>
</tr>
<tr>
<td>Pb</td>
<td>0.027</td>
</tr>
<tr>
<td>As</td>
<td>0.0064</td>
</tr>
<tr>
<td>Si</td>
<td>0.021</td>
</tr>
</tbody>
</table>

### 2D structure of N-(5,6-diphenyl-4,5-dihydro-1,2,4-triazin-3-yl)-guanidine (NTG).
(NMR) spectrometer was used for NMR measurements (DMSO-d$_6$ as solvent, TMS as reference). Infrared spectra were recorded on Nicolet Magna-IR 550 spectrometer with a potassium bromide (KBr) disc in the range from 400 to 4000 cm$^{-1}$. Echem Analyst 4.0 Software was used for plotting, graphing and fitting data. Accelrys and Hyperchem (Version 8.03) software for molecular dynamics simulation and quantum chemical calculations, respectively have been used as described elsewhere [21].

3. Results and discussion

3.1. Weight loss measurements

Corrosion rates of copper coupons were calculated by considering the total affected sample area and immersion times. The average corrosion rates, expressed in mg m$^{-2}$ h$^{-1}$, rare shown in Table 3. Table 3 presents the results of weight loss measurements for the corrosion of copper in 0.5 M H$_2$SO$_4$ solutions devoid of and containing different concentrations of the NTG.

The weight loss of copper coupons in 0.5 M H$_2$SO$_4$ without and with the addition of NTG was used to calculate the inhibition efficiency $\Omega$ (%) by using the following equation:

$$\Omega (%) = \frac{W_0 - W}{W_0} \times 100$$

where $W_0$ and $W$ are the weight loss of copper coupons in sulphuric acid solutions without and with the addition of NTG, respectively.

Inspection of the data in Table 3 reveals that the addition of NTG decreases markedly the corrosion rate of copper. This result indicates the inhibitive effect of the added NTG on copper corrosion in the acidic solution. The inhibition efficiency increases as the concentration of added NTG is increased.

3.2. Potentiodynamic polarization measurements

The pure sulphuric acid and inhibitor-containing sulphuric acid solutions used in this study were all aerated. Theoretically, copper cannot displace hydrogen from acid solutions according to the theories of chemical thermodynamics [22]. However, this situation will change in aerated sulphuric acid. Dissolved oxygen may be reduced on copper surface and this will allow some corrosion in the aerated sulphuric acid solutions at potentials near the corrosion potentials, according to Smyrl [23].

Fig. 2 shows typical anodic and cathodic potentiodynamic polarization curves carried out at 303 K in aerated 0.5 M H$_2$SO$_4$ in the absence and presence of various concentrations of NTG. Electrochemical potentiokinetic parameters are calculated from the polarization curves and presented in Table 4. These electrochemical parameters include corrosion potential ($E_{corr}$), corrosion current density ($i_{corr}$) determined by extrapolation of the anodic Tafel lines, anodic Tafel slope ($\beta_a$) and inhibition efficiency $\Pi$ (%) up to $E_{corr}$ were calculated from the following equation:

$$\Pi (%) = \left(1 - \frac{i_{corr}}{i_{corr}^{ref}}\right) \times 100$$

where $i_{corr}$ and $i_{corr}^{ref}$ are corrosion current densities in absence and presence of NTG, respectively.

Values of the anodic Tafel line slope ($\beta_a$) of 20 mV/decade are consistent with anodic current, depending on diffusion of cupric ions. In case where the anodic Tafel line slope is less than 30 mV/decade, diffusion of cupric ions is suggested [24]. Since it has been found here that the anodic Tafel slope remains almost constant and close to 20 mV/decade, diffusion can be considered to be present and dominant. Because of the addition of NTG, the corrosion rate decreases and the cathodic Tafel slopes should increase in the presence of NTG. That is confirmed from the $E_{corr}$ shifts cathodically and it indicates that NTG affects the cathodic processes [25].

As can be seen in Fig. 2, it was not possible to evaluate the cathodic Tafel slope as there is no visible linear region that prevents linear extrapolation to $E_{corr}$ of the cathodic polarization curves. This irregularity was confirmed by other researchers and can be explained as the superposition of at least two cathodic current contributions: one arises from oxygen reduction and the second one consequential of copper ion re-deposition [26–28]. It is common practice and it was possible in this case to evaluate $j_{corr}$ by extrapolation of the anodic polarization curves only to $E_{corr}$. At more cathodic potential with respect to $E_{corr}$ the characteristic horizontal line resulting from limiting current density for oxygen reduction can be observed.

Also, Fig. 2 shows three clear regions: region (I) that appeared in anodic curve for the copper electrode were the active dissolution (apparent Tafel region), region (II) the transition region, and region (III) the limiting current region. The anodic polarization curve of copper showed a monotonic increase of current with potential in the blank solution. The anodic dissolution of copper in acid medium can be described as follows:

$$2Cu + H_2O \rightarrow Cu_2O + 2H^+ + 2e$$  \hspace{1cm} (5)

$$Cu_2O + 2H^+ \rightarrow 2Cu^{2+} + H_2O + 2e$$  \hspace{1cm} (6)

The cathodic corrosion reaction in an aerated acidic solution is

$$O_2 + 4H^+ + 4e \rightarrow H_2O$$  \hspace{1cm} (7)
The cathodic curves close to the corrosion potential for blank can be ascribed to the reduction of dissolved oxygen present in the test solution. The increase in current density seen at a potential more negative than 820 mV (SCE) is due to hydrogen evolution. This behaviour is similar to that reported by Tromans and Ahmed [29].

On addition of different concentrations of NTG, both the cathodic and anodic current densities were greatly decreased. Table 4 shows that NTG has good inhibiting effect on the corrosion of copper in 0.5 M sulphuric acid and the inhibiting efficiency of NTG increases with the increasing of its concentrations.

### 3.3. Electrochemical impedance spectroscopy

There is a general agreement in the literature that copper corrosion in aerated sulphuric acid exhibited a Warburg impedance in case of short immersion times [30] (5 min to 2 h) and at low frequencies (\( f \leq 10 \) mHz). This diffusion tail (Warburg impedance) disappears at long immersion times and higher frequencies. The appearance of the Warburg impedance at the corrosion potential in aerated sulphuric acid should be attributed to oxygen transport from the bulk solution to the copper surface. Fig. 3 depicts a typical Nyquist plot for inhibitive effect of NTG on copper corrosion in aerated 0.5 M \( \text{H}_2\text{SO}_4 \) in the absence and the presence of NTG.

Fig. 3 depicts a typical Nyquist plot for inhibitive effect of NTG on copper corrosion in aerated 0.5 M \( \text{H}_2\text{SO}_4 \) at the corresponding rest potentials and at 303 K.

The obtained impedance spectrum seems quite reasonable in comparison with those obtained under similar conditions [26]. This suggests similar characteristics of surface layers. The electrode impedance of NTG was higher compared with that in blank solution.

### Table 5

<table>
<thead>
<tr>
<th>NTG concentration (M)</th>
<th>( R_1 ) ( \Omega ) cm(^2)</th>
<th>( R_2 ) ( \Omega ) cm(^2)</th>
<th>CPE/( \mu F ) cm(^{-2})</th>
<th>( n )</th>
<th>( \Psi ) (%)</th>
<th>( \theta_1 )</th>
<th>( \theta_2 )</th>
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<tbody>
<tr>
<td>0</td>
<td>3.2</td>
<td>588</td>
<td>39.5</td>
<td>0.83</td>
<td>--</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>10(^{-4})</td>
<td>3.9</td>
<td>1032</td>
<td>33.2</td>
<td>0.84</td>
<td>43.19</td>
<td>0.43</td>
<td>0.42</td>
</tr>
<tr>
<td>5 \times 10(^{-4})</td>
<td>5.1</td>
<td>1177</td>
<td>20.4</td>
<td>0.92</td>
<td>50.16</td>
<td>0.50</td>
<td>0.49</td>
</tr>
<tr>
<td>10(^{-3})</td>
<td>3.9</td>
<td>2102</td>
<td>11.3</td>
<td>0.93</td>
<td>72.16</td>
<td>0.72</td>
<td>0.73</td>
</tr>
<tr>
<td>5 \times 10(^{-3})</td>
<td>4.5</td>
<td>3925</td>
<td>5.2</td>
<td>0.93</td>
<td>85.10</td>
<td>0.85</td>
<td>0.84</td>
</tr>
<tr>
<td>10(^{-2})</td>
<td>2.9</td>
<td>11773</td>
<td>1.5</td>
<td>0.93</td>
<td>95.01</td>
<td>0.95</td>
<td>0.95</td>
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</table>
Data from Table 5 reveal that, by increasing the concentration of NTG the corrosion rate (1/R_{ct}) decreases. The decrease in CPE values can be attributed to a decrease in dielectric constant and/or an increase in the thickness of the electrical double layer, suggests that the inhibitor molecules act by adsorption mechanism at copper/acid interface [33].

3.4. Adsorption isotherm

The increase in the inhibition efficiencies of copper in 0.5 M H_2SO_4 solutions, with increasing additive concentrations of NTG can be explained on the basis of additive adsorption. This adsorptive behaviour of a corrosion inhibitor is an important part of its study, as they can provide important clues to the nature of the copper–NTG interaction.

![Fig. 4. Equivalent circuit model for NTG, R_s solution resistance, R_{ct} charge transfer resistance and CPE constant phase element.](image)

![Fig. 5. Measured and simulated Nyquist impedance spectra obtained from copper electrode in 0.5 M H_2SO_4 at 303 K.](image)

![Fig. 6. Measured and simulated Nyquist impedance spectra obtained from copper electrode in 0.5 M H_2SO_4 solutions in presence of 10^{-3} M NTG at 303 K.](image)

In the present medium, the additive was seen to follow the Langmuir adsorption isotherm as seen in Fig. 7 according to the following equation:

\[
\frac{1}{\theta} - \theta = KC
\]  

(10)

where \( K \) is the equilibrium constant, \( C \) the NTG concentration which should be expressed in molar units and \( \theta \) is the degree of surface coverage. As \( \theta \) is a dimensionless quantity, \( K \) must have the inverse dimension of concentration. The surface coverage (\( \theta \)) can be calculated from any of the methods used to calculate corrosion inhibition efficiency or arithmetic average of them (\( \theta \)) [34]. In this study in order to fit more accurately, averages of the surface coverage (\( \theta \)) were used. Surface coverages are calculated by the following equations:

\[
\theta_1 = \frac{\Omega}{100}
\]

(11)

\[
\theta_2 = \frac{\Pi}{100}
\]

(12)

\[
\theta_3 = \frac{\Psi}{100}
\]

(13)

where \( \theta \) in Table 5, is the arithmetic average of surface coverage obtained from the three methods.

Fig. 7 shows linear relationship for Eq. (10) with correlation coefficient \( R^2 = 0.94 \) for NTG. It should be explained that other adsorption isotherms (Frumkin and Temkin) were checked and Langmuir adsorption isotherm is the best approximate between them. This is why the assumption is true for Langmuir adsorption isotherm.

Adsorption of NTG on copper surface can be achieved by two modes of adsorption, through the free lone pairs on nitrogen atoms as well as the protonated species of NTG as they are present in acidic medium, nitrogen atoms accept protons from the acid solution and form cations which electrostatically attracted to the pre-adsorbed sulphate anions on copper surface.

At low NTG concentrations its inhibition efficiency is low. This can be explained as there is a partial diffusion control of copper oxidation. That means, for low inhibitor concentrations the inhibition efficiencies are limited not only by the partial coverage of the electrode surface (adsorbed NTG) but also by the diffusion of species in the solution. This is possibly why the above correlation coefficients in Fig. 7 for NTG deviated from 1.
3.5. Molecular simulation

Molecular simulation study was performed to simulate the adsorption structure of the NTG in an attempt for understanding the interactions between NTG and copper surface. Molecular structure of NTG shows that it is likely to adsorb on copper surface by sharing the electrons of nitrogen atoms, phenyl rings and triazine structure with copper. The adsorption progress of NTG on copper surface is investigated by performing molecular mechanics (MM) using MS Modeling Software. The periodic boundary conditions (PBC) were applied to the simulation cell and described elsewhere [21]. All NTG molecules were energy optimized, copper surface and water layers was constructed using the amorphous cell module, the whole system was energy optimized and the possibility of NTG adsorption on the copper surface were simulated as in Fig. 8. It could be seen from Fig. 8 that NTG molecule move near to the copper surface, indicating that NTG adsorbed at copper surface. Fig. 8 shows that there are three different aromatic structures in NTG; one of them (phenyl ring) is out of plane while the other couple of aromatic structures are parallel to the copper surface. Fig. 8 also shows that the adsorption occurred through the nitrogen atoms in NTG. During simulation, both in plane aromatic structures are fluctuating up and down the copper surface while - and - groups are attached all the time to copper surface.

These findings confirm the adsorption of NTG on copper surface with interaction energy calculated from molecular dynamics simulation and equals \(-24.5\ \text{kJ/mol}\).

3.6. Quantum chemical calculations

It is understood that computational methods have a potential application towards the design and development of organic corrosion inhibitors in corrosion field.

In order to investigate the charge distribution of NTG molecule, quantum chemical calculations were performed by Hyperchem 8.0 package. The Mulliken charge distributions of NTG molecule as well as the highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbital (LUMO) were calculated and presented in Fig. 9.

It is confirmed that the more negative the atomic partial charges of the adsorbed centre are, the more easily the atom attracted to the metal surface.

Table 6 shows some of the key quantum chemical parameters were computed using the PM3-SCF method. These are mainly the energies of the highest occupied ($E_{\text{HOMO}}$) and lowest unoccupied molecular orbitals ($E_{\text{LUMO}}$) and total energy ($E_{\text{tot}}$). These quantum chemical parameters were obtained after geometric optimization with respect to the all nuclear coordinates.
Frontier orbital theory is useful in predicting adsorption centers of the inhibitor molecules responsible for the interaction with surface metal atoms [35,36]. Moreover, the gap between the LUMO and HOMO energy levels of the molecules was another important factor that should be considered. Reportedly, excellent corrosion inhibitors are usually those organic compounds who are not only offer electrons to unoccupied orbital of the metal, but also accept free electrons from the metal [37].

It is well established in the literature that the higher the HOMO energy of the inhibitor, the greater the trend of offering electrons to unoccupied d orbital of the metal, and the higher the corrosion inhibition efficiency. In addition, the lower the LUMO energy, the easier the acceptance of electrons from metal surface, as the LUMO–HOMO energy gap decreased and the efficiency of inhibitor improved. Quantum chemical parameters listed in Table 6 reveal that NTG has high HOMO and Low LUMO with high energy gap.

The number of transferred electrons (\(\Delta N\)) was also calculated depending on the quantum chemical method as in the following equation:

\[
\Delta N = \frac{X_Cu - X_{inh}}{2(\eta_{Cu} + \eta_{inh})}
\]

where \(X_Cu\) and \(X_{inh}\) denote the absolute electronegativity of copper and the inhibitor molecule, respectively; \(\eta_{Cu}\) and \(\eta_{inh}\) denote the absolute hardness of copper and the inhibitor molecule, respectively. These quantities are related to electron affinity (\(A\)) and ionization potential (\(I\)) which are useful in their ability to help predict chemical behaviour [38].

\[
\chi = \frac{I + A}{2}
\]

\[
\eta = \frac{I - A}{2}
\]

\(I\) and \(A\) are related in turn to \(E_{HOMO}\) and \(E_{LUMO}\)

\[
I = -E_{HOMO}
\]

\[
A = -E_{LUMO}
\]

Values of \(\chi\) and \(\eta\) were calculated by using the values of \(I\) and \(A\) obtained from quantum chemical calculation. Using a theoretical \(\chi\) value of 4.48 eV/mol according to Pearson’s electronegativity scale and \(\eta\) value of 0 eV/mol for copper [39], \(\Delta N\), is the fraction of electrons transferred from inhibitor to the copper surface, was calculated. Values of \(\Delta N\) showed inhibition effect resulted from electrons donation. Agreeing with Lukovits’s study [40], if \(\Delta N < 3.6\), the inhibition efficiency increased with increasing electron-donating ability at the metal surface. In this study, NTG was the donor of electrons, and the copper oxide surface was the acceptor. NTG was bound to the copper oxide surface, and thus formed inhibitive adsorption layer against corrosion.

The vertical distance, calculated from molecular dynamics, between the flat molecules and copper surface was about 3.2 Å for NTG; this result indicates that the interaction between the NTG molecules and the copper surface is very strong.

4. Conclusions

The main conclusions of the present study can be summarized as follows:

1. The measurements demonstrated that under the chosen experimental conditions NTG offer sufficient protection against copper corrosion in 0.50 M H₂SO₄ solutions.
2. Tafel polarization studies have shown that the NTG suppresses the cathodic process and thus it acts as cathodic-type inhibitor.
3. The results of EIS indicate that the value of CPEs tends to decrease and both charge transfer resistance and inhibition efficiency tend to increase by increasing the inhibitor concentration. This result can be attributed to increase of the thickness of the electrical double layer.
4. Molecular dynamic simulations are performed to investigate the adsorption behaviour of NTG on copper surface.
5. The relationship between efficiency of inhibition efficiency of copper in 0.5 M H₂SO₄ and the \(E_{HOMO}, E_{LUMO} = E_{HOMO}\) and \(\Delta N\) of NTG were calculated by PM3-SCF method.

Acknowledgement

The author acknowledges Prof. Reda Mohammady Abdel-Rahman (D.Sc.) for preparation of the inhibitor.

References


Table 6

Simulated and quantum chemical parameters for NTG

<table>
<thead>
<tr>
<th>Calculated parameters for NTG</th>
<th>Value</th>
</tr>
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<tbody>
<tr>
<td>Adsorption energy (kJ/mol)</td>
<td>-24.5</td>
</tr>
<tr>
<td>(E_{HOMO}) (eV)</td>
<td>-9.096732</td>
</tr>
<tr>
<td>(E_{LUMO}) (eV)</td>
<td>-0.857793</td>
</tr>
<tr>
<td>(\Delta (E_{LUMO} - E_{HOMO})) (eV)</td>
<td>8.3238</td>
</tr>
<tr>
<td>(-E_{inh}) (kJ/mol)</td>
<td>300882.2</td>
</tr>
<tr>
<td>Dipole moment (D)</td>
<td>4.841</td>
</tr>
<tr>
<td>(\Delta N)</td>
<td>0.06</td>
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