IRAQI Academic Scientific Journals

Samarra Journal of Pure and Applied Science

SJPAS

www.sjpas.com

ISSN:2663-7405

Prediction the effect of the most efficient factors on the adsorption process of some azo dyes compounds on carbon surface using quantum mechanical methods

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Article Information

Received: 31/12/2019
Accepted: 26/01/2020

Keywords:

Quantum mechanics, adsorption, azo dyes

Abstract

This work includes the adsorption study of four azo dyes. The used dyes are *p*-COOH RD, *m*-NO_2 RD, *p*-Br RD, and *p*-NH_2 RD. The study aims to determine the most efficient sites of the dyes that connect to the surface of the adsorbent to understand the mechanism of removing these dyes from contaminated water. The calculations have been achieved using quantum mechanics methods including two semiempirical methods AM1, PM3, and Ab initio (HF). The total energy of the molecule 18.167 kcal., the energies of HOMO -3.060 ev and LUMO -5.357 ev, the energy gap between them, hardness, and atomic charges have been calculated. The obtained results show that the nitrogen atoms in the azo dyes are the most influencing factor affect the adsorption process. By comparing the practical results with the theoretical ones, it was found that the azo group the most efficient group on the stability of these compounds and responsible for the adsorption of the studied compounds.

Introduction

AZO dyes are complex organic compounds containing the active group R-N = N-R (R alkyl group or aryl group) [1]. AZO dyes have wide applications in multiple fields such as optics [2], textile industry [3], fast food [4] and cosmetics [5]. Despite its many benefits and various applications, the azo dyes are contaminants by discharging them into water, as they are liquid wastes harmful to human health [6]. Due to inefficient dyeing, 10-15% of dyes are lost in effluents during dyeing [7]. Azo dyes are an environmental concern due to the aromatic intermediate compounds resulting from their biodegradation [8]. Therefore, the removal of these dyes from wastewater has great importance. One of the most important methods used is adsorption [9].

This research is based on the theoretical study of four azo dyes consisting of the association of aniline compensators with the resorcinol ring. The main sites in the structure of dyes affecting the adsorption efficiency of these dyes on different adsorbent surfaces are studied. The quantum chemical methods and molecular drawing technique are able to define a large number of molecular properties, efficiency, geometry, and substation groups on the molecular. The use of theoretical methods has two positive advantages; first, many

compounds can be distinguished based on their molecular structure, second, determination of reaction mechanism through knowledge of the chemical effectiveness of compounds [10].

The information calculated by quantum mechanics methods differs from practically measured quantities regardless of natural interference as opposed to experimental measurements. There is no statistical error in quantum chemistry calculations. If an error is found, it is inherent and is associated with the assumptions required to facilitate calculations [11]. There are several methods in quantum mechanics:

1. Semi-empirical methods

These methods are based on the approximation of the Schrödinger equation in the calculations, some integrals are compensated by practical values rather than calculated. In the past decades, semi-experimental methods have been widely used, the Austin AM1 method is one of the most recent methods developed by Michael Dewar Associates in 1985 [12]. This method depends on the neglect of interference between the two atoms. In addition, there is PM3 method developed by Stuart in 1989 [13]. Semi-experimental methods can be applied to different directions, as the MNDO [14]. AM1, PM3 method is designed to study the heat composition and synthesis of a large number of organic molecules. Other semi-empirical methods (INDO/CNDO) are concerned with the study of spectral characteristics.

2. Ab initio methods

The term Ab initio refers to the fact that calculations and data are preliminary and there is no empirical data. They include a solution for all mathematical integrals and thus face difficulties arising from the large number of integrals that requires it to be made, that is, it is not a valid solution to the Schrödinger equation, but it works on the use of a limited number of physical attributes in its computation such as electron charge. Planck's constant and the speed of light, which use many derivatives and integrals to find approximate solutions to the Schrödinger equation. Therefore, finding the kinetic and thermodynamic values that are close to real values [14]. One of the most basic methods used is Hatree-Fock HF. Functions calculated by using quantum mechanics methods:

Atomic charges

Chemical bonds are either polar or covalent bonds. Atomic charges are responsible for electrostatic reactions. Electronic density and atomic charges are important in many chemical reactions and the physical and chemical properties of compounds. Atomic charge of molecules is used as evidence of chemical activity and as a measure of the strength of molecular interference, and it controls the interconnection between the atom and its adjacent atom. There are many methods to calculate charges, the most famous of which is the Millikan method [15], used in calculating the distribution of charges in the molecule and this method provides an explanation of the composition and effectiveness of molecules.

Molecular orbital energies

These orbitals determine the way a molecule interacts with another molecule and includes highest Occupied Molecular Orbital Energy (EHOMO) and lowest unoccupied Molecular Orbital Energy (ELUMO), HOMO acts as an electron donor. The lowest energy LUMO, which has sufficient space to receive electrons, is the receiver of electrons. According to the theory of molecular orbital, the transition state is due to the interference between the HOMO and LUMO orbit of the reactants [16]. The HOMO energy is directly related to the

ionization potential and the LUMO energy is directly related to the electron affinity and the HOMO-LUMO gap, i.e. the difference in energy between the HOMO and LUMO. Another term, SOMO, represents the term in the case of a single electron in the compound if the compound is a free radical [17].

Materials and methods

The used materials in adsorption are activated charcoal, kaolin, Ethanol 99 %, KOH 10 % and HCl 0.1N, the used materials in the preparation of dyes are aniline, *m*-nitro aniline, *p*-amino aniline, *p*-amino benzoic acid, *p*-bromo aniline and *p*-hydroxy aniline.

Preparation of azo dyes

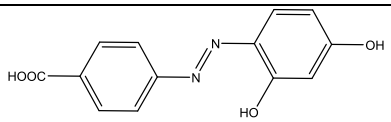
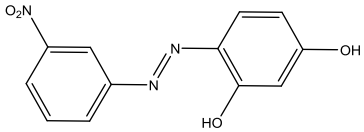
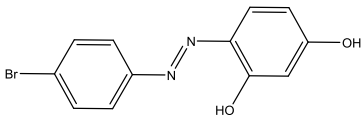
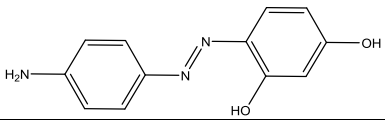
First: Preparation of diazonium salt

Dissolved 2 g meta-nitro-aniline in 12 ml concentrated hydrochloric acid in baker. Placed the thermometer in the solution and immersed the baker in a bath of ice powder. Cool with stirring until the temperature is below 5 °C. Dissolved 1 g of sodium nitrite in 5 ml distilled water and cool the solution by submerging it in the ice bath 0-5 °C. Added sodium nitrite solution in batches 1-2 ml per batch to the solution prepared in cold step 1, stirring and maintain the temperature so that the temperature in the reaction mixture does not exceed 5 ° C.

Second: Preparation of azo dye

Prepared a solution of 3 g of resorcinol dissolved in 9 ml 10% sodium hydroxide solution. Cool the solution with an ice bath to less than 5 °C by adding ice to the reaction mixture. Stir the resorcinol solution, and then added the prepared diazonium solution in the first step. Red crystals separated from the dye. Placed the final solution in an ice bath for an hour to stabilize the solution. Filtrate using a filter funnel, washing the crystals with distilled water and then leave to dry in the oven at 50 °C. The previous steps are used to prepare the remaining dyes. Table 1 shows the dyes and their properties that were prepared and studied in this paper.

Table 1: Prepared dyes and their properties

Dyes	Structure formula of dye	Color	Melting Point (° C)	λ max, (nm)
p-COOH RD		Orange yellow	168-170	392
m-NO_2 RD		Red	178-176	386
p-Br RD		Red	150-152	387
p-NH_2 RD		Reddish brown	179-177	388

Study of adsorption

Adsorption was studied by changing the concentration of dyes adsorbent while keeping all other variables constant, amount of adsorbent 0.05 gm and the temperature and shaking speed constant 80 rpm and when the natural acidity of the solution of each dye was done according to the following steps:

- Apply in five dry flasks 10 ml of the dye solution of concentrations (5×10^{-4} M, 3×10^{-4} M, 1×10^{-4} M, 7×10^{-5} M, 5×10^{-5} M), respectively, and 0.5 gm of adsorbent (activated charcoal, kaolin clay) is added.
- Shaked the solutions for 60 minutes in volumetric flasks of 50 ml at a speed of 80 rpm and at a temperature 25 °C.
- The solutions were then filtered and the amount of adsorbed material was estimated using UV spectrum.

Theoretical part

Chem office is one of the most efficient programs in completing traditional and advanced calculations, which provides researchers with the means to support scientific research by providing a number of calculates methods in theoretical chemistry, as well as giving broad perceptions and options in this field, the calculations in the field of quantum chemistry are carried out in this research using (Chem office 3D) and (Chem draw CD) to draw molecules.

The (AM1, PM3, and HF) methods were used to study the four dyes shown in Fig. 1, because these dyes are similar in composition and differ in substituted groups on the ring only, so it was selected, to study the effect of different substituted groups on the adsorption efficiency [18]. After drawing, the compound molecule and conducting the process of energy reduction minimize energy using the program (MM2). The molecular interference represented by the total energy of the molecule was calculated, each of the above methods was used to calculate charges existing molecular on the nitrogen atoms of the azo bond, the ionization voltage of the molecules is also calculated, and orbital energies LUMO and HOMO through which the hardness of the molecule was calculated by the following equation [19]:

$$\eta = 1/2\ [\text{ELUMO} - \text{EHOMO}] \quad (1)$$

The value of electronic chemical potential [M] is calculated using the equation below:

$$M = 1/2\ [\text{ELUMO} + \text{EHOMO}] \quad (2)$$

The calculation of the value of the global electrophilicity index, which is symbolized by W, can be applied by the following equation:

$$W = [\ M2/2\eta\ ] \quad (3)$$

Although semi-empirical and because of the approximations they use are less accurate than Ab initio calculate ions, they are more widely used.

Results and discussion

Practical part

The method used to accomplish this study by using the spectral method. This must be determined the most appropriate concentration of the study with a specific amount of activated charcoal and Kaolin clay in order to reach equilibrium with the color remaining in solution. It does not make sense to use concentrations and quantities of the adsorbent surface in which the process of decolorization is complete. The equilibrium state was reached by studying the range of concentrations of dyes (5×10^{-5}-7×10^{-7} M).

This study was accomplished by shaking a certain volume 10 ml of the dye solution at a constant temperature of 25 °C, using an amount of activated charcoal 0.05 g and at the natural acidic function of the solution of each dye, this process was repeated using the same quantities and concentrations with kaolin, the solutions were shaken for an hour and then filtered. Absorbance was measured and the residual concentration was calculated. The adsorption percentage and adsorption capacity were estimated using on the following equations:

$$ads.\% = \frac{Ci - Ce}{Ci} \times 100 \qquad (4)$$

$$qe = \frac{Ci - Ce}{m} \times V \qquad (5)$$

Whereas:

qe adsorption capacity (mg/g)
Ci initial concentration (mg/L)
Ce residual concentration at equilibrium (mg/L)
m quantity of adsorbent (gm)
V is the volume of the solution used (L)

The obtained results are listed in the tables 2 and 3.

Table 2: The effect of the initial concentration on the adsorption capacity using activated charcoal as an adsorbent at a constant temperature 293 K and at the natural acidic function of each dye and 60 minutes time.

Dyes	qe (mg/g) at conc. M × 10^{-4}				
	5	3	1	7	5
p-COOH RD	22.04	14.02	4.71	3.31	2.36
m-NO_2 RD	21.3	13.87	4.42	3.33	2.38
p-Br RD	28.72	15.7	5.28	3.59	2.68
p-NH_2 RD	19.37	12.08	4.36	2.86	2.05

Table 3: The effect of the initial concentration on the adsorption capacity using Kaolin as an adsorbent at constant temperature 293 K and at the natural acidic function of each dye and 60 minutes time.

Dyes	qe (mg/g) at conc. M × 10^{-4}				
	5	3	1	7	5
p-COOH RD	15.48	8.25	2.88	2.47	2.01
m-NO_2 RD	15.27	10.92	3.62	3.004	2.23
p-Br RD	19.33	11.62	3.96	3.006	2.16
p-NH_2 RD	12.75	9.98	3.34	2.39	1.75

It can be noticed that the adsorption capacity increases with increasing concentration at a constant temperature; this can be explained by the fact that increased concentration facilitates the transfer of mass to the surface of the adsorbent. In subsequent studies, the concentration (3×10^{-4} M) was adopted as an intermediate state in terms of the effect on adsorption capacity and retention of color presence. If the adsorption capacity of the dyes studied at concentration (5×10^{-4} M) is compared and the temperature is 298 K, and using activated charcoal as an adsorbent surface it is observed to increase in the following sequence:

p-NH_2 < *m*-NO_2 < *p*-COOH < *p*-Br (28.72 < 22.04 < 21.3 < 19.37) respectively.

To explain this behavior of dyes, the dyes were compared in terms of composition i,e the presence of different substituted groups (puller or impulse) which affect through the inductive factor on the presence of electronic abundance on the two charcoal atoms in the azo group which is responsible for the adsorption by binding them. The composition of the dyes is in the form of two ends, one constant is the ring resorcinol, and the second part represents

benzene ring substituted by different substitutions in terms of their inductive drag and electronic payment.

It was observed that the dye containing an electron-pulling group had a greater adsorption capacity than the dye containing the driving group. This is due to the fact that the puller group makes the spread of electronic current wider on all the dye composition. While the impulse group limits the spread of electrons on the dye structure due to electron repulsion. Because these groups reduce the electronic affinity for the ring, thus the stability of the potential complex on the surface decreases.

Theoretical part

1. Geometry optimization method

The total energy of each dye molecule can be calculated from the sum of the structural abnormalities in which the result of bonding in the molecule to the torsion, stretched and bending. As well as the forces of a space disability and forces of electrostatic repulsion-attraction calculate the interference caused by the spatial distribution of the molecule between non-bonded atoms intertwined.

Calculate the total energy of a molecule from the interference set as shown by:

$$\text{Total energy} = \text{Stretching energy} + \text{Bending energy} + \text{Torsion energy} + \text{Non bonded interaction energy} \quad (6)$$

The total energy represented by the sum of the forces mentioned in the equation for the dye molecules is calculated and is listed in table 4.

Table 4: Values of the energies of the structural deformities resulting from the spatial interference represented by the total energy.

Dyes	Stretch	Bend	S.T.B	Torsion	non-1,4 VDW	1,4 VDW	Dipole/ dipole	Total energy	qe
p-COOH RD	1.1988	7.6800	0.0206	-9.5000	-1.1190	14.7879	5.0992	18.1675	14.70
m-NO_2 RD	0.9241	6.1860	0.0665	-11.1566	0.5503	15.7282	0.6303	7.7426	14.03
p-Br RD	0.7630	5.6706	0.0593	-11.1600	-1.0452	13.9237	0.2442	8.4557	16.23
p-NH_2 RD	0.7399	5.5736	0.0398	-13.2800	-1.1365	12.7875	0.1588	4.8832	12.32

The stretched energy in the table is due to the distance of the bonds from the standard lengths of the bonds involved. The energy of bending or angular tension represents a departure from the optimal angle values for hybridization. Tensile energy represents the energy created between atoms separated by three bonds, i.e. how far away they are from the diffraction position between adjacent atoms. For non-bonded interference, the Vanderfalls interference group represents either attraction or repulsion, and electrostatic interference that arises between charges, dipole and quadrupole.

When comparing the values of the adsorption capacity (qe) obtained at 60 min, the natural acidity of the dye solution and the temperature of 298 K at 3×10^{-4} M. The adsorption capacity is proportional to the energies that control the geometry and stability of the molecule, this increase is in the direction of increasing the total energy, ie decreasing the

stability of the molecule and thus increasing the adsorption capacity, in other words, the less stable molecule in solution is more it tends to bind to the surface of the adsorbent. The optimal stereo obtained for dyes is shown in figure 1.

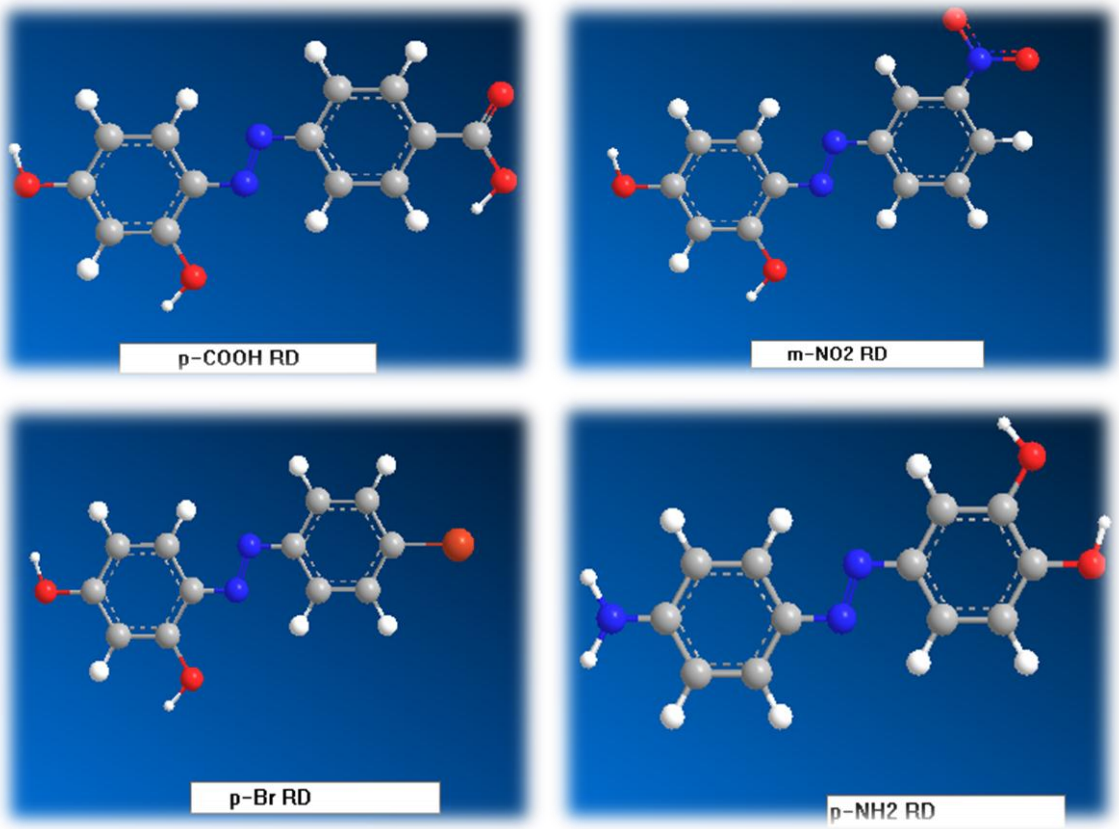


Fig. 1: The optimal stereo obtained for dyes

2. Atomic charges

The aim of this study is to find the binding set of the dye molecule with the adsorbent surface and the possibility of determining the nature of the binding forces. The adsorption process results from the attraction between the charges on the solid surface is formed by the distribution of the heterogeneous surface pores, a difference in energy is generated and these charges interact with the charges generated on the dye. This study used several methods of quantum mechanics to calculate atomic charges. The charges for nitrogen atoms on the azo bond for the dyes are calculated in the table 5.

Table 5: Muliken charges for nitrogen atoms in each dye by AM1, PM3, HF

Dyes	Muliken charge		
	AM1	PM3	HF
p-COOH RD	N(8) -0.0269 N(7) -0.0956	N(8) 0.0364 N(7) -0.0644	N(8) -0.3597 N(7) -0.4084
m-NO_2 RD	N(8) -0.0287 N(7) 0.0916	N(8) 0.0348 N(7) -0.0582	N(8) -0.3619 N(7) -0.4076
p-Br RD	N(80 -0.0306 N(7) -0.0940	N(8) 0.0262 N(7) -0.0588	N(8) -0.3614 N(7) -0.4054
p-NH_2 RD	N(8) -0.0495 N(7) -0.0812	N(8) 0.0078 N(7) -0.0415	N(8) -0.3819 N(7) -0.4063

From the observation of atomic charge values on nitrogen atoms in the azo bond of the dyes under study which are most likely to be responsible for binding to the surface of the adsorbent [20]. It was found that the electronic density and the values of charges on the nitrogen atom [7], close to the substituted ring more than the nitrogen atom [8], close on the ring resorcinol.

3. Stability of the dyes

A theoretical study was carried out to determine the stability of the dyes under study by finding some variables related to stability. The energy gap between the orbitalis (LUMO) and (HOMO) gives an indication of the molecule stability. To find the correlation pattern between dye stability and adsorption capacity values, LUMO and HOMO values were calculated according to the three theories AM1, PM3, and HF. The results are listed in the table 6.

Table 6: Values of HOMO and LUMO for the dyes under study and according to the three theories

Dyes	Theory	LUMO ev	HOMO ev	LUMO - HOMO
	AM1	-3.060	-5.357	2.297
p-COOH RD	PM3	-3.044	-5.015	1.971
	HF	-3.442	-4.884	1.442
	AM1	-3.072	-4.506	1.434
m-NO_2 RD	PM3	-3.108	-4.364	1.256
	HF	-3.448	-4.506	1.058
	AM1	-2.998	-3.831	0.833
p-Br RD	PM3	-3.164	-3.694	0.53
	HF	-3.408	-3.745	0.345
	AM1	-3.006	-3.459	0.453
p-NH_2 RD	PM3	-3.099	-3.465	0.366
	HF	-3.254	-3.444	0.19

A simple comparison of the adsorption capacity values (qe) gives the following in table 7:

Table 7: Adsorption capacity values (qe)

Theory	*p*-COOH RD	*m*-NO_2 RD	*p*-Br RD	*p*-NH_2 RD
AM1	2.297	1.434	0.833	0.453
PM3	1.971	1.256	0.53	0.366
HF	1.442	1.058	0.345	0.19
Qe	14.70	14.03	16.23	12.32

The study indicates that the lower stability dye gives greater adsorption on the surface. The values of η, M and w for all dyes were calculated using the three theories and results were obtained which are listed in the table 8.

Table 8: Values of η, M and w for all dyes using the three theories

Dyes	Theory	η	M	W
	AM1	1.1485	-4.2085	7.710
p-COOH RD	PM3	0.9855	-4.029	8.237
	HF	0.721	-4.163	12.018
	AM1	0.717	-3.789	10.011
m-NO_2 RD	PM3	0.628	-3.736	11.112
	HF	0.529	-3.977	14.949
	AM1	0.416	-3.410	13.966
p-Br RD	PM3	0.265	-3.429	22.184
	HF	0.177	-3.576	36.133
	AM1	0.226	-3.232	23.117
p-NH_2 RD	PM3	0.183	-3.282	29.430
	HF	0.095	-3.349	59.026

Analysis of the results listed in the above table, which includes the values of hardness and electron affinity and evidence of spherical electrophilic presence of solvent. The calculations show the following order of particle rigidity:

p-COOH RD > m-NO_2 RD > *p*-Br RD > *p*-NH_2 RD

Since the hardness is proportional to the stability of the molecules [21], the *p*-COOH RD dye was more stable, but both m-NO_2 RD and *p*-Br RD are of less stability the stability, This difference in stability comes from the difference of the substituted groups where the NH_2 group in p-NH_2 RD gave the lowest stability compared to other dyes. Hardness is also associated with the energy gap between LUMO and HOMO and by increasing the energy gap, chemical reactions are highly stable. As well as linked to molecular polarization, ie, the reduction of the energy gap leads to the so-called easier polarization of the molecule [22]. On the other hand, a molecule with a lower hardness value behaves as a nucleophile this corresponds to the values of the atomic charge, which in turn correspond to the values of adsorption capacity Which determines the atom (site) from which the adsorbent surface can bind to the dye.

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IRAQI Academic Scientific Journals

Samarra Journal of Pure and Applied Science

SJPAS

ISSN:2663-7405

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تقصي التنبؤ بأثر العوامل الأكثر كفاءة على عملية امتزاز بعض مركبات أصباغ الآزو على سطح الكربون باستخدام طرائق مكانيك كم مختلفة

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معلومات البحث:

تأريخ الاستلام: 2019/12/31

تأريخ القبــول: 2020/01/26

الكلمات المفتاحية:

ميكانيك الكم، الامتزاز، أصباغ الآزو

الخلاصة:

شمل البحث دراسة امتزاز أربعة أصباغ ازو، وكانت الأصباغ المستخدمة هي p-COOH RD و $m\text{-}NO_2$ RD و p-Br RD و $p\text{-}NH_2$ RD ، تهدف الدراسة إلى تحديد أكثر المواقع كفاءة للأصباغ التي تتصل بسطح المادة الماصة لفهم آلية إزالة هذه الأصباغ من المياه الملوثة. تم تحقيق الحسابات النظرية باستخدام طرق ميكانيكا الكم بما في ذلك طريقتان شبه تجريبية semiempirical هما Am1 وPM3، وطريقة من طرق الحسابات الأساسية Ab initio وهي HF. تم حساب إجمالي الطاقة للجزيء 18.167 kcal وطاقات HOMO - 5.357ev و LUMO -3.060ev وفجوة الطاقة بينهما، والصلابة، والشحنة الذرية. أظهرت النتائج التي تم الحصول عليها أن ذرات النيتروجين في أصباغ الآزو هي العامل الأكثر تأثيرًا في عملية الامتزاز. بمقارنة النتائج العملية بالنتائج النظرية، وجد أن مجموعة الآزو هي المجموعة الأكثر كفاءة في ثبات هذه المركبات والمسؤولة عن امتزاز المركبات التي تمت دراستها.