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Synthesis, Analytical and Theoretical Studies of (*Z*)-4-amino-3-hydroxy-2-((4-(*N*-(5-methylisoxazol-3-yl)Sulfamoyl)Phenyl)Diazenyl)Naphthalene-1-Sulfonic Acid

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Abstract

New azodye that characterize (*Z*)-4-amino-3-hydroxy-2-((4-(*N*-(5-methylisoxazol-3-yl) sulfamoyl) phenyl)diazenyl)naphthalene-1-sulfonic acid (1) was synthesized. The azodye has been characterized by IR, visible spectra and elemental (CHN) analysis. The results of visible spectra which recorded in the range (360-6540) nm were showed that the maximum wave length (λmax) of azodye was 500 nm. Analytical studies carried on the dye, the results of the solvent effect were showed high solubility in ethanol and water. But, the results of the pH effect in a range of buffer solution were gave three isopestic points. The ionization constant (pKa) and protonation constant (pKb) were calculated by using the half height method. The results were showed that the pKp1 and pKp2 of each nitrogen atom and pKa of OH-group were equal to 2.5, 4.5 and 8.5 respectively. Theoretical studies also carried on azodye (1). The actual and optimal bonds length of -N=N- was equal to 1.248 in each. Though, internal coordinate mechanics (ICM) of (1) was showed that the angle type in most of atoms was dihedral. But, the *R* and *S* configuration were observed in other atoms in the structure of azodye. The results also indicated that the torsion angles (ψ) of (1) were variable. High close contacts of atoms were observed in the structure of azodye. The molecular mechanics (MM2) properties was intended for (1), the results showed that the stretch, bend, stretch-bend, torsion, non-1,4 VDW, 1,4 VDW and the total energy were equal to 61.0809, 627.0240, -1.6517, 179.0634, 4686.8146, 33.0379 and 5585.3692 kcal/mol respectively. High VDW interactions of this molecule was observed, due to the results of dipole/dipole were not computed. Thus, the result of MM2 minimization for azodye (1) was showed high VDW interactions of this molecule higher than before the minimization, due to the result of dipole/dipole was also not computed. The high steric energy (1235.782) was affecting the results of minimization. However, the results of the molecular mechanics force field (MMFF94) energy and gradient for azodye (1) were showed that the total energy and RMS gradient were equal to 26223.422 kcal/ mol and 9113.745 respectively. Further, the results of MMFF94 minimization and MMFF94 minimization/sampling of azodye (1) were showed that the minimization was attended successfully using this method.

Keywords: Internal coordinate, Molecular mechanics, Azodyes

1. Introduction

Azo compounds were receiving high attention in scientific research,1 they have great importance in chemical analysis. A strongly colored compound can be yellow, red, orange, blue or even green, depending on the exact structure of the molecule due to make azo compounds as extremely importance as dyes and also as pigments for a long time.2 The structural features in organic compounds, that usually produce color are C=C, N=O, N=N, aromatic rings, C=O and NO_2. Though, the groups that always confer color are the azo (–N=N–) and nitroso (–N=O) while the other groups actually do so under certain conditions.3 Azo dyes contain one or more azo groups (–N=N–) which are linked to SP_2 hybridized carbon atoms, based on the number of such groups.4 These compounds contain more than one active group, which is able to formulate chelatic coordinational complexes with metal ions distinguished by their color and ability to dissolve in different solvents.3

Internal coordinates are an attractive alternative to the Cartesian coordinates of each atom when particular degrees of freedom are not of interest.5 Internal coordinates such as bond lengths, bond angles, and torsion angles are natural coordinates for describing a bonded molecular system.6 It has recently been suggested by Mu *et al.* [Proteins 58, 45 2005)] to use backbone dihedral angles instead of Cartesian coordinates in a principal component analysis of molecular dynamics simulations. Dihedral angles may be advantageous because internal coordinates naturally provide a correct separation of internal and overall motion, which was found to be essential for the construction and interpretation of the free energy landscape of a biomolecule undergoing large structural rearrangements.7 which describe the essential physics of a biomolecular process such as protein folding or molecular recognition.3 Molecular modeling can be considered as a range of computerized techniques based on theoretical chemistry methods and experimental data that can be used either to analyse molecules and molecular systems or to predict molecular, chemical, and biochemical properties.8 One of the major advantages of molecular mechanics compared to other computational techniques is the relative ease with which structures can be optimized via minimization of the corresponding potential energy functions.9 The area of molecular mechanics is to study the detailed structure and physical properties of molecules. Molecular mechanics calculates the energy of a molecule and then adjusts the energy through changes in the bond lengths and angles to obtain the minimum energy structure. Internal coordinate also have some advantages for suggesting a new derivatives.10

Thomas11 introduced MMFF94, the initial published version of the MMFF. It describes the objectives set for MMFF, the form it takes, and the range of systems to which it applies. This study also outlines the methodology employed in parameterizing MMFF94 and summarizes its performance in reproducing computational and experimental data.

2. Result and discussion

The new azodye which characterize (*Z*)-4-amino-3-hydroxy-2-((4-(*N*-(5-methylisoxazol-3-yl) sulfamoyl) phenyl) diazenyl) naphthalene-1-sulfonic acid (1) was synthesized, (Figure 1).

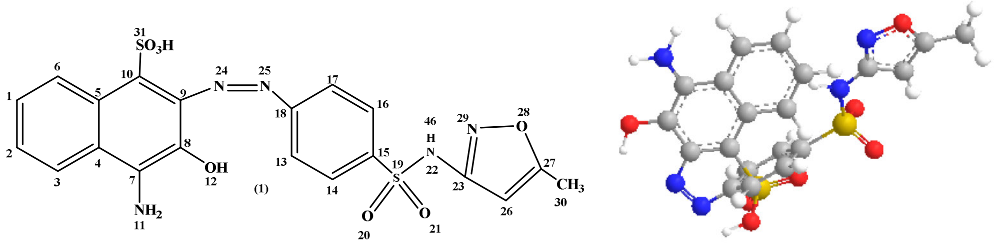


Figure (1): The (*Z*)-4-amino-3-hydroxy-2-((4-(*N*-(5-methylisoxazol-3-yl)sulfamoyl)phenyl)di azenyl) naphthalene-1-sulfonic acid (1).

The IR spectrum was showed a broad peak at 3300-3450 cm^{-1} for the O–H stretch. It can be concluded that the OH group may form a hydrogen bond with nitrogen atom. The results were also showed that the azodye (1) was having two absorption bands at 3300–3410 cm^{-1} region which may attribute to the -NH_2 group, which overlaps with the stretching of the OH group. Though, the band corresponding to N=N stretching was appeared at 1455 cm^{-1}, but the C=C stretching of the aromatic ring shows a strong band at 1500 cm^{-1} region. The stretching of aromatic C-H was appeared at 2900 cm^{-1}. The azodye (1) was also characterized by elemental analysis, (C, 47.71; H, 3.40; N, 13.91; O, 22.24; S, 12.73). Though, the effect of solubility of orange azodye (1) was studied in a range of solvents. The results were showed high solubility in 45 mL of ethanol and 5 mL of water. Thus, the pH effect was also studied for 8*10-5 M solution of (1) in a range of buffer solution at pH (1-12), (Figure 2). The results were showed that the suitable pH values found to be in the range of (1-8). Three isopestic points were also presented in Figure (2) below.

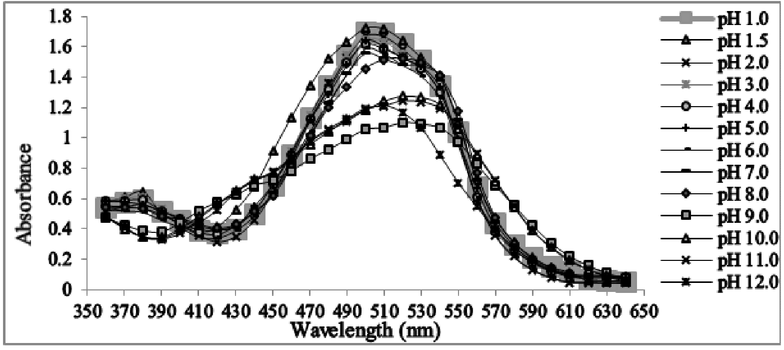


Figure 2: The pH effect of azodye (1).

The pKa of hydroxyl group and pKb of the nitrogen atom in azodye (1) were calculated by applying the half height method.12 From this method the pK values were attained using equation (1) and (2) below. This method was depending on the fact that the limiting absorption (Al) represents complete the conversion of one form to other. Since pK is equal to pH at which the two forms exist in equivalent amount, then the pH corresponding to half the height of the absorbance, the pH curve is equal to pK.

pK= pH (at A1/2) ……………………… (1)

A1/2= (Al + Amin)/ 2 …………………… (2)

The pK (at A1/2) of azodye (1) was intended from the absorbance-pH curve in figure (3) below.

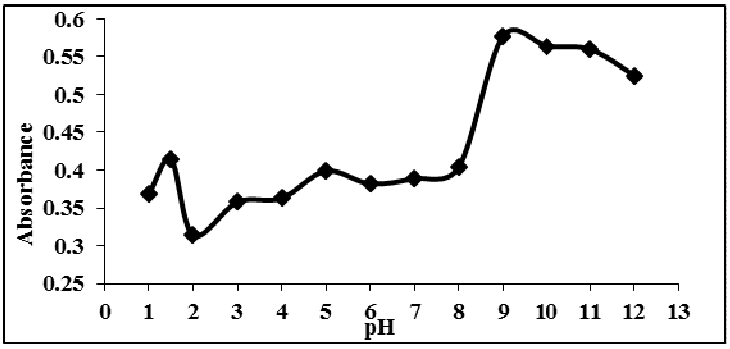


Figure 3: Absorbance-pH effect of azodye (1) at λ_{420} nm.

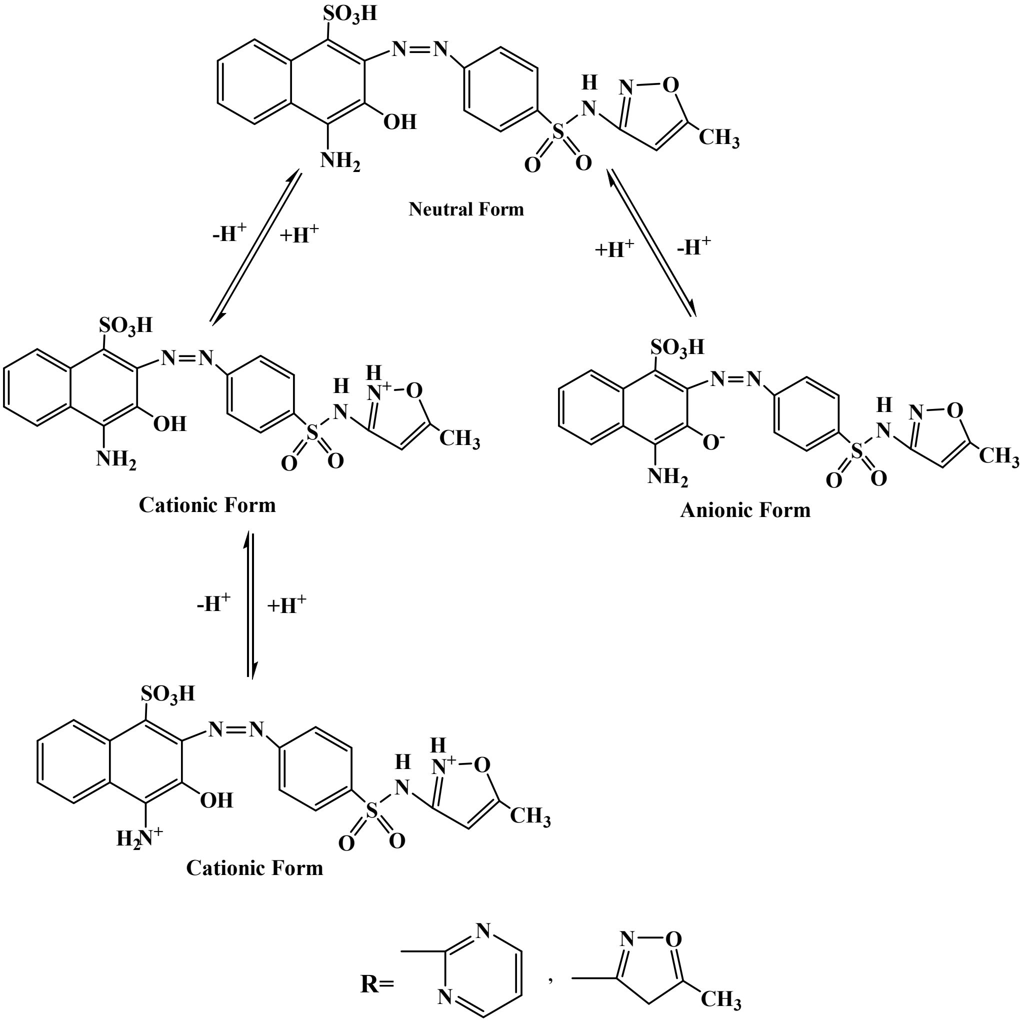
The results obtained are given in table (1) below.

Table (1): Spectrophotometric determination of ionization and protonation constants of azodye

pK_{p1}	pK_{p2}	pK_a	λ (nm)
2.5	4.5	8.5	420

pKp1= Protonation of the nitrogen atom.
pKp1= Protonation of the nitrogen atom.
pKa= Ionization of the OH-group.

The absorption spectra, (Figure 2) of azodye (1) in the varying pH values, (1-12) are explained in Scheme (1) below. The results indicate the existence of the following equilibrium scheme of which displays the suggested ionization of azodye in acidic and basic medium.12



Scheme (1): The suggested ionization of azodye (1) in acidic and basic medium.

Analysis of azodye (1) was studied theoretically. The results were showed that the exact mass and the abundance of $C_{20}H_{17}N_5O_7S_2$ (1) were equal to 503.0569 and 69.74% respectively. Thus, the actual and optimal bond lengths between atoms in (1) were also intended hypothetically, (Table 2).

Table (2): The selected bonds length of azodye (1)

Atoms	Actual	Optimal
O(34)-H(51)	0.942	0.942
S(31)-O(34)	1.660	-
S(31)-O(33)	1.450	1.450
S(31)-O(32)	1.450	1.450
C(30)-H(48)	1.113	1.113
O(28)-N(29)	1.387	-
C(27)-O(28)	1.357	1.323
C(27)-C(30)	1.497	1.497
C(26)-H(47)	1.100	1.100
C(27)-C(26)	1.370	1.420
N(25)-N(24)	1.248	1.248
C(23)-C(26)	1.406	1.420
N(29)-C(23)	1.335	1.358
N(22)-H(46)	1.050	1.050
N(22)-C(23)	1.266	1.462
S(19)-N(22)	1.696	-
S(19)-O(20)	1.450	1.450
N(25)-C(18)	1.260	1.456
C(17)-C(18)	1.395	1.420
S(19)-C(15)	1.790	-
C(14)-C(15)	1.395	1.420
O(12)-H(41)	0.972	0.972
N(11)-H(40)	1.050	1.050
C(10)-S(31)	1.790	-
C(9)-N(24)	1.260	1.456
C(8)-O(12)	1.355	1.355
C(7)-N(11)	1.266	1.462
C(4)-C(5)	1.414	1.420
C(3)-C(4)	1.404	1.420

The table shows that the actual and optimal bonds length of -N=N- was equal to 1.248 in each. Thus, the ICM for azodye (1) were also calculated as seen in table (3) below.

Table (3): The internal coordinate mechanics of azodye (1)

No	Atom	Bond Atom	Bond Length (Å)	Angle Atom	Angle (^{o})	2nd Angle Atom	2nd Angle (^{o})	2nd Angle Type
1	C(1)							
2	C(2)	C(1)	1.392					
3	C(3)	C(2)	1.396	C(1)	119.996			
4	H(36)	C(2)	1.1	C(1)	120.003	C(3)	120.002	Pro-R
5	C(4)	C(3)	1.404	C(2)	120.741	C(1)	-0.008	Dihedral
6	H(37)	C(3)	1.1	C(2)	119.63	C(4)	119.63	Pro-R
7	C(5)	C(4)	1.414	C(3)	119.266	C(2)	0.009	Dihedral
8	C(7)	C(4)	1.404	C(3)	121.464	C(5)	119.27	Pro-S
9	C(6)	C(1)	1.396	C(2)	119.986	C(3)	0.004	Dihedral
10	C(10)	C(5)	1.404	C(4)	119.264	C(6)	121.47	Pro-R
11	H(35)	C(1)	1.1	C(2)	120.007	C(6)	120.007	Pro-S
12	H(38)	C(6)	1.1	C(1)	119.627	C(5)	119.627	Pro-S
13	C(8)	C(7)	1.396	C(4)	120.738	C(3)	-179.998	Dihedral
14	N(11)	C(7)	1.266	C(4)	119.632	C(8)	119.631	Pro-S
15	C(9)	C(10)	1.396	C(5)	120.747	C(4)	-0.001	Dihedral
16	O(12)	C(8)	1.355	C(7)	120.003	C(9)	120.003	Pro-S
17	N(24)	C(9)	1.26	C(8)	120.006	C(10)	120.008	Pro-R
18	S(31)	C(10)	1.79	C(5)	119.627	C(9)	119.626	Pro-S
19	N(25)	N(24)	1.248	C(9)	107.498	C(8)	180	Dihedral
20	C(18)	N(25)	1.26	N(24)	107.501	C(9)	0	Dihedral
21	C(13)	C(18)	1.395	N(25)	119.999	N(24)	-90	Dihedral
22	C(17)	C(18)	1.395	C(13)	120	N(25)	120.001	Pro-S
23	C(14)	C(13)	1.395	C(18)	120.003	C(17)	-0.001	Dihedral
24	H(42)	C(13)	1.1	C(14)	119.998	C(18)	119.999	Pro-R
25	C(15)	C(14)	1.395	C(13)	119.997	C(18)	0.006	Dihedral
26	H(43)	C(14)	1.1	C(13)	120.001	C(15)	120.001	Pro-S
27	C(16)	C(17)	1.395	C(18)	119.997	C(13)	-0.003	Dihedral
28	S(19)	C(15)	1.79	C(14)	120	C(16)	120	Pro-R
29	H(44)	C(16)	1.1	C(15)	119.998	C(17)	119.998	Pro-S
30	H(45)	C(17)	1.1	C(16)	120.002	C(18)	120.001	Pro-R
31	N(22)	S(19)	1.696	C(15)	109.462	C(14)	119.999	Dihedral
32	O(20)	S(19)	1.45	C(15)	109.442	N(22)	109.52	Pro-R
33	O(21)	S(19)	1.45	C(15)	109.5	O(20)	109.442	Pro-R
34	C(23)	N(22)	1.266	S(19)	120	C(15)	-180	Dihedral
35	H(46)	N(22)	1.05	S(19)	120	C(23)	120	Pro-S
36	C(26)	C(23)	1.406	N(22)	123.96	S(19)	0	Dihedral
37	N(29)	C(23)	1.335	N(22)	123.96	C(26)	112.08	Pro-R
38	C(27)	C(26)	1.37	C(23)	103.824	N(22)	-180	Dihedral
39	H(47)	C(26)	1.1	C(23)	128.088	C(27)	128.088	Pro-R
40	O(28)	N(29)	1.387	C(23)	105.247	N(22)	-179.999	Dihedral
41	C(30)	C(27)	1.497	C(26)	125.196	O(28)	125.195	Pro-R
42	O(34)	S(31)	1.66	C(10)	109.462	C(5)	120	Dihedral
43	O(32)	S(31)	1.45	C(10)	109.5	O(34)	109.462	Pro-R
44	O(33)	S(31)	1.45	C(10)	109.442	O(32)	109.442	Pro-R
45	H(39)	N(11)	1.05	C(7)	120	C(4)	180	Dihedral
46	H(40)	N(11)	1.05	C(7)	120	H(39)	120	Pro-R
47	H(41)	O(12)	0.972	C(8)	108.001	C(7)	179.999	Dihedral
48	H(48)	C(30)	1.113	C(27)	109.5	C(26)	-180	Dihedral
49	H(49)	C(30)	1.113	C(27)	109.441	H(48)	109.442	Pro-S
50	H(50)	C(30)	1.113	C(27)	109.462	H(48)	109.462	Pro-R
51	H(51)	O(34)	0.942	S(31)	120	C(10)	59.977	Dihedral

The table demonstrates the effect of the configuration in the results of internal coordinate and indicated that the results of ψ angles of azodye (1) were variable. Further, the close contacts of atoms in (1) were also calculated as seen in table (4) below.

Table (4): The close contacts of atoms in azodye (1)

No	Atoms	Close contact atoms	No	Atoms	Close contact atoms
1	H(45)-H(51)	1.505	51	C(1)-S(19)	2.361
2	C(17)-H(51)	1.822	52	C(13)-C(16)	2.79
3	C(18)-H(51)	1.957	53	S(31)-C(16)	1.823
4	N(25)-H(51)	1.812	54	H(38)-C(16)	1.701
5	H(37)-H(40)	1.708	55	C(10)-C(16)	2.293
6	H(42)-O(33)	1.395	56	C(6)-C(16)	2.2
7	C(14)-O(33)	2.17	57	C(5)-C(16)	2.449
8	C(17)-O(33)	2.646	58	S(31)-H(43)	2.872
9	C(13)-O(33)	1.131	59	C(18)-C(15)	2.79
10	C(18)-O(33)	1.557	60	S(31)-C(15)	2.036
11	N(25)-O(33)	2.104	61	H(38)-C(15)	0.607
12	H(44)-O(32)	2.356	62	C(10)-C(15)	2.506
13	S(19)-O(32)	2.514	63	C(6)-C(15)	1.568
14	C(16)-O(32)	1.472	64	C(5)-C(15)	2.324
15	H(43)-O(32)	2.356	65	C(1)-C(15)	2.754
16	C(15)-O(32)	1.016	66	S(31)-H(42)	2.305
17	C(14)-O(32)	1.472	67	C(10)-H(42)	2.585
18	C(17)-O(32)	2.106	68	C(17)-C(14)	2.79
19	C(13)-O(32)	2.106	69	S(31)-C(14)	1.823
20	C(18)-O(32)	2.360	70	H(38)-C(14)	1.701
21	H(38)-O(32)	1.618	71	C(10)-C(14)	2.292
22	C(6)-O(32)	2.533	72	C(6)-C(14)	2.200
23	H(45)-O(34)	1.346	73	C(5)-C(14)	2.449
24	C(16)-O(34)	2.294	74	S(31)-C(17)	1.298
25	C(17)-O(34)	1.253	75	C(9)-C(17)	2.61
26	C(18)-O(34)	1.732	76	C(10)-C(17)	1.792
27	N(25)-O(34)	2.183	77	C(5)-C(17)	2.682
28	S(19)-H(47)	2.666	78	S(31)-C(13)	1.298
29	H(35)-N(29)	2.397	79	C(9)-C(13)	2.61
30	S(19)-C(26)	2.915	80	C(10)-C(13)	1.792
31	H(35)-C(26)	2.459	81	C(5)-C(13)	2.682
32	H(35)-H(46)	1.445	82	S(31)-C(18)	0.929
33	C(6)-H(46)	1.891	83	C(9)-C(18)	2.006
34	C(2)-H(46)	2.065	84	C(10)-C(18)	1.48
35	C(1)-H(46)	1.246	85	C(5)-C(18)	2.791
36	H(35)-C(23)	1.494	86	S(31)-N(25)	2.117
37	C(1)-C(23)	2.448	87	C(10)-N(25)	2.333
38	H(38)-O(20)	2.348	88	N(24)-S(31)	2.948
39	H(35)-O(20)	2.326	89	H(38)-S(31)	2.563
40	H(38)-N(22)	2.3	90	C(6)-S(31)	3.044
41	H(35)-N(22)	0.942	91	O(12)-N(24)	2.701
42	C(6)-N(22)	2.198	92	N(11)-O(12)	2.7
43	C(2)-N(22)	2.674	93	C(4)-C(9)	2.81
44	C(1)-N(22)	1.534	94	H(37)-N(11)	2.471
45	S(31)-H(45)	2.305	95	C(3)-N(11)	2.765
46	C(10)-H(45)	2.585	96	C(5)-C(8)	2.809
47	S(31)-H(44)	2.872	97	C(7)-C(10)	2.787
48	H(38)-S(19)	1.443	98	C(3)-C(6)	2.787
49	H(35)-S(19)	1.986	99	C(2)-C(5)	2.81
50	C(6)-S(19)	2.131	100	C(1)-C(4)	2.81

The table displays high close contacts of atoms in the structure of azodye (1). Thus, the MM2 properties was also intended for azodye (1), the results were showed that the stretch, bend, stretch-bend, torsion, non-1,4

VDW, 1,4 VDW and total energy were equal to 61.0809, 627.0240, -1.6517, 179.0634, 4686.8146, 33.0379 and 5585.3692 kcal/mol respectively. High VDW interactions of this molecule was observed, due to the results of dipole/dipole were not computed. Thus, the results of MM2 minimization for azodye (1) were showed that the stretch, bend, stretch-bend, torsion, non-1,4 VDW, 1,4 VDW and total energy were equal to 282.9677, 313.9823, 10.3424, 138.7782, 451.9570, 37.7542 and 1235.7819 kcal/ mol respectively. Higher VDW interactions of this molecule were observed after minimization, due to the result of dipole/dipole was also not computed. The high steric energy (1235.782) was affecting the results of and the RMS Gradient after minimization was equal to 0.010.

The MMFF94 energy and gradient for azodye (1) were also intended. The results were showed that the total energy and RMS gradient for this frame were equal to 26223.422 kcal/ mol and 9113.745 respectively. Thus, the MMFF94 minimization iteration which is terminated normally because the gradient norm is less than the minimum gradient norm was also envisioned. The results were showed that the final energy was equal to 1032.86 kcal/ mol. However, the results of MMFF94 minimization/sampling which calculated for azodye (1) were showed that the final energy was equal to 1032.97 kcal/ mol. These results also displayed that the minimization was attended successfully.

3. Excremental section

Asodye (1) was synthesis by a method similar to that described by Fox.13 This dye was prepared as following:

1. The 4- amino-N-(5-methyl-3-isoxazoyl)-benzenesulfonamide (0.006 mole, 1.5197 g) was dissolved in 2.1 mL of conc. HCl followed by adding 5 mL of distilled water. The mixture was stirrer and was kept in ice bath.
2. The $NaNO_2$ (0.456 g) was dissolved in about 10 mL of distilled water and also was kept in ice bath.
3. Diazonium salt was prepared by adding sodium nitrite solution in step (2) dropwise to the cold solution of amine in the step (1) with continue stirring and keep the temperature around 0.5^{o}C.
4. Coupler was prepared by dissolving 1-amino-2-hydroxy naphthalin sulfonic acid (0.006 mole, 2.4200 g) in 25% sodium hydroxide solution and keeping in ice bath.
5. The diazonium salt was added drop wisely to the coupler with constant stirring, keeping the temperature around 0.5^{o}C, the dye were neutralized with dilute hydrochloric acid solution.
6. The resulting crudes were recrystallized from methanol to yield orange compound (4.5 g, 94%); M.P= 236 ^{o}C. This azodye has been characterized by IR in the range (4000–600) cm^{-1} as KBr discs, and visible spectra (λ_{max}= 500 nm) and CHN analysis.

Summary

This study focused in area of synthesis a new azodye which followed by analytical and theoretical studies. The later concentrated in the MM2, in order to study the detailed structure and physical properties of the molecule. MM2 calculates the energy of a molecule and then adjusts the energy through changes in the bond lengths and angles to obtain the minimum energy structure. Also, the ICM results were gave some advantages for suggesting new derivatives.

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