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Synthesis, characterization and DFT computational studies of new heterocyclic azo compounds

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ABSTRACT

New heterocyclic azo compounds were prepared by coupling the diazonium salts with *N*-(4-methylphenyl)maleimide with various different sulfa compounds. The structure of heterocyclic azo compounds was determined by MS, FT-IR and ^{1}H NMR techniques. The density function theory calculation at the B3LYP method with 6-311G(d,p) basis set is used to investigate the electronic structures of the prepared heterocyclic azo compounds. Mulliken charge distributions and HOMO-LUMO energies of the mentioned compounds have been also computed by same method and basis set.

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1. Introduction

Azo compounds acquired wide interest in application to biological system [1]. In pharmaceuticals, azo linkage was used to protect drug from undesirable reaction, such as prontosil was found to protect against, and cure streptococcal infections in mice. Interestingly prontosil was inactive on bacterial cultures. Prontosil is totally in active *in vitro* but possesses excellent activity *in vivo* [2,3]. The azo compounds are applicable in biocidal treatment of textile materials because they exhibit biological activity [4]. Azo compounds are well known for their medicinal importance and are recognized for their applications as antiseptics, antidiabetics, antibacterial, and antitumor [5-10]. Azo compounds are also involved in a many biological reactions such as carcinogenesis, protein synthesis and inhibition of DNA [11-15]. In the chemical industry, aromatic azo compounds are widely used as pigments [16], food additives, indicators, [17] radical reaction initiators [18] and therapeutic agents [19]. Moreover, azo compounds considered promise in electronics [20] and drug delivery [21]. The first effective antibacterial drugs that could be used systemically for the cure of bacterial infection in humans were containing the azo sulfonamides compounds [22].

The present paper reports on the synthesis of a series of heterocyclic azo compounds containing the sulfonamide functional group. The chemical structures of the heterocyclic azo compounds were studied using spectral methods and theoretical calculations.

2. Experimental

2.1. Instrumentation

All the chemicals were used as received without further purification except for aniline, was distilled before use. FT-IR spectra were measured at room temperature using a Perkin-Elmer 2000 FT-IR equipped with a high-purity dried potassium bromide (KBr) beam splitter. The ^{1}H NMR spectra were obtained using a Bruker 400 MHz NMR spectrometer with tetramethylsilane as the internal reference. The mass spectra were recorded on a Perkin Elmer Clarus 500 Gas Chromatography-Mass Spectrometry system (GC-MS).

2.2. Synthesis

2.2.1. Preparation of N-(4-methylphenyl)maleimide (I)

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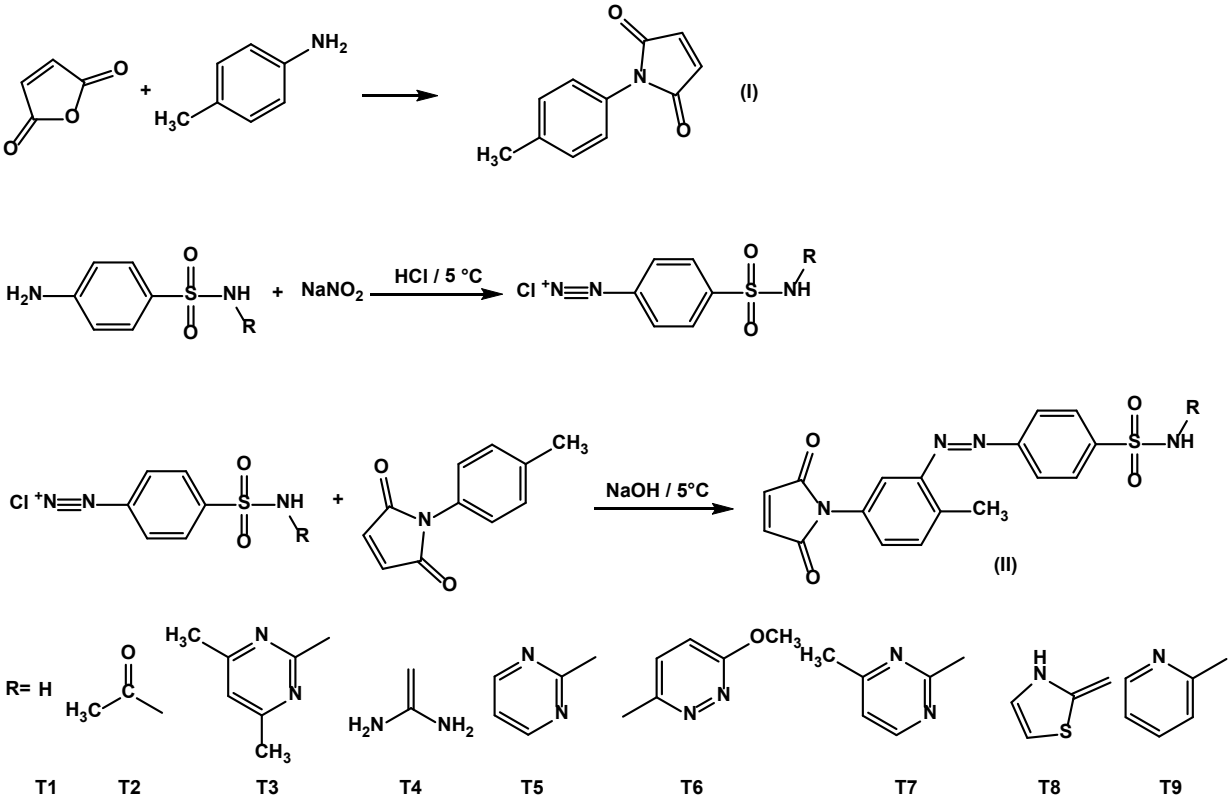

Scheme 1

4-Methyaniline (0.15 mol) and maleic anhydride (0.15 mol) were dissolved separately in DMF (50 mL) to yield solutions A and B, respectively (Scheme 1). Solution B was added dropwise into solution A to give solution C. Solution C was stirred for 2 hours at 20 °C in a water bath. P_2O_5 (12 g) was dissolved in H_2SO_4 (10 mL) and DMF (70 mL). This mixture was added dropwise into solution C and was stirred for 2 hours at 70 °C. The mixture was kept chilled in the ice bath and poured into cold water. A precipitate formed that was filtered, washed with distilled water and finally recrystallized from 2-propanol and dried in a vacuum oven at 65 °C for 24 hours. M.p.: 151-153 °C [23].

2.2.2. General procedure for preparation of the heterocyclic azo compounds (T1-T9)

Solution A was prepared by mixing sulfa compounds (0.01 mol) with concentrated HCl (0.3 mL) and water (2 mL) and cooling at 5 °C in an ice bath. $NaNO_2$ (0.69 g, 0.01 mol) was dissolved in water (2 mL) at 5 °C to obtain solution B. Then solution A was added dropwise to solution B at 5 °C with stirring. The mixture was then slowly added into the solution of *N*-(4-methylphenyl)maleimide (0.01 mol), which was dissolved in 10% NaOH (2 mL) at 5 °C. The mixture was keep chilled in the ice bath and stirred continuously for 10 min. The precipitate formed was filtered and recrystallized from ethanol and hexane in ratio (4:6). The procedure was repeated by substituted different sulfa compounds (Scheme 1).

4-((5-(2, 5-Dioxo-2, 5-dihydro-1H-pyrrol-1-yl)-2-methylphenyl)diazenyl)benzenesulfonamide (**T1**): Color: Light brown. Yield: 70%. M.p.: 176-178 °C. FT-IR (KBr, ν, cm^{-1}): 3275 (N-H), 3095 (C-H Arom.), 2924 (C-H Aliph.), 1705 (C=O), 1635 (C=C), 1533 (N=N), 1161, 1327 (SO_2), 1288 (C-N). ^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): 2.31 (s, 3H, CH_3-Ph), 4.45 (s, 2H, CH=CH), 6.29 (s, 2H, Ar-H), 6.48 (s, 2H, Ar-H), 7.13 (d, *J* = 7.5 Hz, 1H, Ar-H), 7.50 (dd, *J* = 7.5, 1.5 Hz, 1H, Ar-H), 7.52 (s, 1H, Ar-H), 10.41 (s, 2H, NH_2). MS (EI, *m/z* (%)): 370 (M^+, 100).

N-((4-((5-(2, 5-Dioxo-2, 5-dihydro-1H-pyrrol-1-yl)-2-methylphenyl)diazenyl)phenyl)sulfonyl)acetamide (**T2**): Color: Brown. Yield: 65%. M.p.: 178-179 °C. FT-IR (KBr, ν, cm^{-1}): 3285 (N-H), 3094 (C-H Arom.), 2924 (C-H Aliph.), 1701 (C=O), 1636 (C=C), 1528 (N=N), 1153, 1329 (SO_2), 1265 (C-N). ^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): 1.93 (s, 3H, CH_3-CO-N), 2.26 (s, 3H, CH_3-Ph), 6.29 (d, *J* = 7.5 Hz, 1H, C*H*-CH), 6.47 (d, *J* = 7.5 Hz, 1H, CH-C*H*), 7.15 (dd, *J* = 7.5, 1.5 Hz, 2H, Ar-H), 7.53 (d, *J* = 7.5 Hz, 2H, Ar-H), 7.95-7.51 (m, 3H, Ar-H), 10.32 (s, 1H, NH). MS (EI, *m/z* (%)): 412 (M^+, 100).

N-(4, 6-Dimethylpyrimidin-2-yl)-4-((5-(2, 5-dioxo-2, 5-dihydro-1H-pyrrol-1-yl)-2-methyl-phenyl)diazenyl)benzenesulfonamide (**T3**): Color: Yellow. Yield: 67%. M.p.: 188-190 °C. FT-IR (KBr, ν, cm^{-1}): 3275 (N-H), 3091 (C-H Arom.), 2918 (C-H Aliph.), 1701 (C=O), 1635 (C=C), 1531 (N=N), 1182, 1327 (SO_2), 1267 (C-N). ^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): 2.25 (s, 6H, Pyr-2CH_3), 2.31 (s, 3H, CH_3-Ph), 7.04 (s, 1H, Pyr-H), 7.46 (d, *J* = 7.5 Hz, 1H, Ar-H), 7.65 (dd, *J* = 7.5, 1.5 Hz, 1H, Ar-H), 7.86 (s, 2H, Ar-H), 8.18-8.09 (m, 5H, Ar-H), 9.00 (s, 1H, NH). MS (EI, *m/z* (%)): 476 (M^+, 100).

N-(Diaminomethylene)-4-((5-(2, 5-dioxo-2, 5-dihydro-1H-pyrrol-1-yl)-2-methylphenyl)di-azenyl)benzenesulfonamide (**T4**): Color: Light yellow. Yield: 58%. M.p.: 184-185 °C. FT-IR (KBr, ν, cm^{-1}): 3284 (N-H), 3093 (C-H Arom.), 2915 (C-H Aliph.), 1701 (C=O), 1635 (C=C), 1523 (N=N), 1183, 1328 (SO_2), 1269 (C-N). ^{1}H NMR (400 MHz, $CDCl_3$, δ, ppm): 2.31 (s, 3H, CH_3-Ph), 7.32 (s, 2H, CH=CH), 7.46 (s, 4H, 2×NH_2), 8.18 (m, 2H, Ar-H), 8.20 (m, 3H, Ar-H), 8.27 (dd, *J* = 7.5, 1.5 Hz, 1H, Ar-H), 8.61 (d, *J* = 7.5, 1.5 Hz, 1H, Ar-H). MS (EI, *m/z* (%)): 412 (M^+, 100).

4-((5-(2,5-Dioxo-2,5-dihydro-1H-pyrrol-1-yl)-2-methylphenyl)diazenyl)-N-(pyrimidin-2-yl)benzenesulfonamide (**T5**): Color:

Light yellow. Yield: 58%. M.p.: 184-185 °C. FT-IR (KBr, ν, cm^{-1}): 3284 (N-H), 3093 (C-H Arom.), 2924 (C-H Aliph.), 1701 (C=O), 1635 (C=C), 1527 (N=N), 1182, 1329 (SO_2), 1267 (C-N). ^1H NMR (400 MHz, $CDCl_3$, δ, ppm): 2.31 (s, 3H, CH_3-Ph), 7.06 (t, *J* = 7.5 Hz, 1H, Pyr-H), 7.46 (d, *J* = 7.6 Hz, 1H, Ar-H), 7.65 (dd, *J* = 7.5, 1.5 Hz, 1H, Ar-H), 7.86 (s, 2H, CH=CH), 8.18-8.09 (m, 5H, Ar-H), 8.58 (d, *J* = 7.5 Hz, 2H, Pyr-H), 9.00 (s, 1H, NH). MS (EI, *m/z* (%)): 448 (M^+, 100).

4-((5-(2,5-Dioxo-2,5-dihydro-1H-pyrrol-1-yl)-2-methylphenyl)diazenyl)-N-(6-methoxy-pyridazin-3-yl) benzenesulfonamide (**T6**): Color: Orange. Yield: 60%. M.p.: 181-183 °C. FT-IR (KBr, ν, cm^{-1}): 3284 (N-H), 3080 (C-H Arom.), 2924 (C-H Aliph.), 1701 (C=O), 1635 (C=C), 1529 (N=N), 1182, 1330 (SO_2), 1264 (C-N). ^1H NMR (400 MHz, $CDCl_3$, δ, ppm): 2.31 (s, 3H, CH_3-Ph), 3.84 (s, 3H, O-CH_3), 7.16-7.06 (m, 2H, Ar-H), 7.46 (d, *J* = 7.6 Hz, 1H, Ar-H), 7.65 (dd, *J* = 7.5, 1.5 Hz, 1H, Ar-H), 7.86 (s, 2H, CH=CH), 8.18-8.09 (m, 3H, Ar-H), 8.58 (d, *J* = 7.5 Hz, 2H, Pyr-H), 9.00 (s, 1H, NH). MS (EI, m/z (%)): 478 (M^+, 100).

4-((5-(2,5-Dioxo-2,5-dihydro-1H-pyrrol-1-yl)-2-methylphenyl)diazenyl)-N-(4-methylpyrimidin-2-yl)benzenesulfonamide (**T7**): Color: Yellow. Yield: 38%. M.p.: 191-192 °C. FT-IR (KBr, ν, cm^{-1}): 3284 (N-H), 3091 (C-H Arom.), 2960 (C-H Aliph.), 1701 (C=O), 1635 (C=C), 1531 (N=N), 1180, 1327 (SO_2), 1267 (C-N). ^1H NMR (400 MHz, $CDCl_3$, δ, ppm): 2.37 (s, 3H, CH_3-Ph), 2.57 (s, 3H, Pyr-CH_3), 7.20 (d, *J* = 7.5 Hz, 1H, Ar-H), 7.46 (d, *J* = 7.6 Hz, 1H, Ar-H), 7.65 (dd, *J* = 7.5, 1.5 Hz, 1H, Ar-H), 7.86 (s, 2H, CH=CH), 8.18-8.09 (m, 4H, Ar-H), 8.88 (d, *J* = 7.5 Hz, 2H, Pyr-H), 9.00 (s, 1H, NH). MS (EI, *m/z* (%)): 462 (M^+, 100).

4-((E)-(5-(2, 5-dioxo-2, 5-dihydro-1H-pyrrol-1-yl)-2-methyl phenyl)diazenyl)-N-((E)-thiazol-2(3H)-ylidene) benzenesulfonamide (**T8**): Color: Light gray. Yield: 55%. M.p.: 180-182 °C. FT-IR (KBr, ν, cm^{-1}): 3284 (N-H), 3091 (C-H Arom.), 2922 (C-H Aliph.), 1701 (C=O), 1635 (C=C), 1527 (N=N), 1143, 1327 (SO_2), 1267 (C-N). ^1H NMR (400 MHz, $CDCl_3$, δ, ppm): 2.38 (s, 3H, CH_3-Ph), 6.10 (d, *J* = 11.0 Hz, 1H, NH-CH=C), 6.86 (d, *J* = 11.0 Hz, 1H, S-CH=C), 7.03 (d, *J* = 10.8 Hz, 1H, Ar-H), 7.18 (d, *J* = 10.8 Hz, 1H, Ar-H), 7.33 (d, *J* = 7.5 Hz, 2H, Ar-H), 7.86 (s, 2H, CH=CH), 8.13-8.08 (m, 2H, Ar-H), 8.21 (dd, J = 7.5, 1.5 Hz, 1H, Ar-H), 10.90 (s, 1H, NH). MS (EI, *m/z* (%)): 453 (M^+, 100).

4-((5-(2,5-Dioxo-2, 5-dihydro-1H-pyrrol-1-yl)-2-methylphenyl)diazenyl)-N-(pyridin-2-yl)benzenesulfonamide (**T9**): Color: Yellow. Yield: 60%. M.p.: 186-189 °C. FT-IR (KBr, ν, cm^{-1}): 3284 (N-H), 3089 (C-H Arom.), 2924 (C-H Aliph.), 1701 (C=O), 1635 (C=C), 1527 (N=N), 1182, 1328 (SO_2), 1267 (C-N). ^1H NMR (400 MHz, $CDCl_3$, δ, ppm): 2.34 (s, 3H, CH_3-Ph), 7.06-6.96 (m, 2H, Ar-H), 7.17 (d, *J* = 11.0 Hz, 1H, Ar-H), 7.32 (d, *J* = 7.5 Hz, 1H, Ar-H), 7.41 (ddd, *J* = 7.5 Hz, 1H, Ar-H), 7.73 (td, *J* = 8.0, 1.3 Hz, 1H, Ar-H), 7.94-8.02 (m, 4H, Ar-H), 8.05 (dd, *J* = 7.5, 1.5 Hz, 1H, Ar-H), 8.41 (dd, *J* = 5.1, 1.2 Hz, 1H, Ar-H), 8.70 (d, *J* = 1.5 Hz, 1H, Ar-H), 9.10 (s, 1H, NH). MS (EI, *m/z* (%)): 447 (M^+, 100).

2.3. Computational details

All computations were performed using the Gaussian09 [24] software package. Full geometry optimizations were carried out using the Density Function Theory at B3LYP level for studied compounds [25,26]. Properties and HOMO-LUMO energies of the studied compounds was calculated by the 6-311+G(d,p) higher basis set level. Mulliken charge distributions of the investigated compounds were also computed at same level of method.

3. Results and discussion

3.1. Synthesis and characterization

The preparation of compounds **T1**-**T9** is shown in Scheme 1. The structure of these compounds was confirmed by FT-IR, ^1H NMR, and Mass spectrum. The most important characteristic band of the IR spectra of the prepared compounds **T1**-**T9** is the appearance of the N-N group at 1523-1533 cm^{-1}. This is a sign of the coupling reaction of the reactive coupling bands at 3022-3095 cm^{-1} are attributed to the stretching vibration of the aromatic C-H, as shown in the bands at 2887-2960 cm^{-1} is attributed to aliphatic C-H, as well as the appearance of bands at 1701-1705 cm^{-1} attributed to two groups C=O, and there is a band at 1143-1327 cm^{-1} due to symmetric and asymmetric stretching vibration of the SO_2 group. The FT-IR data for compounds **T1**-**T9** showed the same characteristic bands of the coupling agents **I** and **II**, namely imide, methyl, group, alkene, and *p*-substituted band while the presence of the azo (N=N) group band in 1533-1523 cm^{-1} range confirmed the success of the synthesis. The ^1H NMR for azo compounds **T2** has been chosen as typical example. In the ^1H NMR spectrum of compound **T2**, the protons of the alkene group (HC=CH) and the protons of aromatic ring appeared at δ 6.48-6.29 ppm and δ 7.13-7.52 ppm, respectively.

3.2. Computational results

3.2.1. Geometrical optimization

The visualization of the optimized geometrical structure and atomic labeling of compound **T1** calculated by the B3LYP method with 6-311+G(d,p) basis set are given in Figure 1.

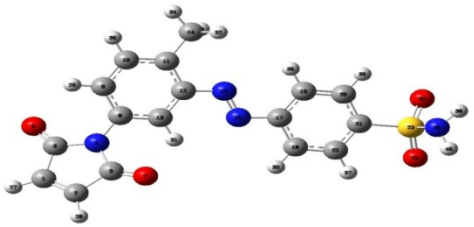

Figure 1. Optimized structures of compound **T1** calculated by the B3LYP method with 6-311+G(d,p) basis set with atom numbering.

3.2.2. Mulliken population analysis

Dipole moment, molecular polarizability and bond properties are affected by atomic charges, therefore, the Mulliken atomic charge calculation has an important role in quantum chemistry [27]. Mulliken population analysis was performed using DFT/B3LYP calculation method with 6-311+G(d,p) basis set for studied compounds. Graphical reorientations of Mulliken charge distributions of studied compounds **T1**-**T9** is shown in Figure 2. As can be seen in Table 1, all the carbon atoms have a net positive charge. The obtained atomic charge shows that the N26 atom (which bonded with different substituted) has lower negative atomic charge (-0.2928) in compounds **T1** and **T2** than the other studied **T3**-**T9** compounds which obtained -0.3133, -0.5415, -0.2958, -0.3140, -0.3055, -0.5182 and -0.2932, respectively. The highest negative atomic charge was -0.5415 in compound **T4**, also compound **T4** has higher negative oxygen atom charge, which obtained -0.5695.

3.2.3. Total energies, dipole moments and molecular orbitals analysis

The HOMO energy represents the ability to donate an electron, LUMO energy as an electron acceptor represents the ability to obtain an electron [27]. The HOMO-LUMO energy calculations of the title compounds were performed using DFT/B3LYP method with 6-311+G(d,p) basis set for the studied compounds **T1**-**T9**.

Table 1. The Mulliken atomic charge distribution of compounds **T1**-**T9**.

Atoms	Mulliken atomic charges (Q/e)								
	Compounds								
	T1	T2	T3	T4	T5	T6	T7	T8	T9
1 C	0.0186	0.0186	0.0162	0.0149	0.0163	0.0174	0.0162	0.0153	0.0170
2 C	0.0189	0.0189	0.0162	0.0161	0.0167	0.0183	0.0165	0.0160	0.0174
3 C	0.4011	0.4011	0.4003	0.4004	0.4004	0.4012	0.4003	0.4004	0.4006
4 N	-0.5172	-0.5172	-0.5158	-0.5154	-0.5159	-0.5168	-0.5159	-0.5154	-0.5164
5 C	0.4003	0.4003	0.3996	0.3993	0.3995	0.3999	0.3997	0.3994	0.3998
6 O	-0.3008	-0.3008	-0.3015	-0.3022	-0.3015	-0.3012	-0.3016	-0.3019	-0.3013
7 O	-0.2973	-0.2973	-0.2972	-0.2967	-0.2970	-0.2972	-0.2969	-0.2970	-0.2969
8 C	0.1547	0.1547	0.1521	0.1517	0.1527	0.1543	0.1526	0.1516	0.1536
9 C	0.0941	0.0941	0.0904	0.0884	0.0909	0.0929	0.0904	0.0889	0.0917
10 C	0.0127	0.0127	0.0104	0.0088	0.0107	0.0120	0.0104	0.0092	0.0114
11 C	-0.0760	-0.0760	-0.0775	-0.0780	-0.0772	-0.0763	-0.0776	-0.0778	-0.0769
12 C	0.0231	0.0231	0.0246	0.0249	0.0245	0.0238	0.0247	0.0248	0.0243
13 C	0.1719	0.1719	0.1701	0.1692	0.1703	0.1706	0.1703	0.1692	0.1706
14 C	0.1456	0.1456	0.1437	0.1409	0.1439	0.1453	0.1436	0.1419	0.1447
15 N	-0.2059	-0.2059	-0.2079	-0.2096	-0.2077	-0.2071	-0.2081	-0.2088	-0.2078
16 N	-0.2045	-0.2045	-0.2043	-0.2038	-0.2043	-0.2046	-0.2039	-0.2038	-0.2042
17 C	0.0506	0.0506	0.0491	0.0450	0.0493	0.0495	0.0487	0.0454	0.0481
18 C	0.0770	0.0770	0.0581	0.0650	0.0624	0.0755	0.0622	0.0660	0.0741
19 C	0.1167	0.1167	0.1074	0.1071	0.1086	0.1116	0.1078	0.1079	0.1141
20 C	0.1074	0.1074	0.1130	0.0905	0.1132	0.1343	0.1119	0.0987	0.1047
21 C	-0.3940	-0.3940	-0.3169	-0.2934	-0.3201	-0.3003	-0.3192	-0.3004	-0.3232
22 C	0.1402	0.1402	0.1570	0.1301	0.1564	0.0950	0.1581	0.1267	0.1239
23 S	1.1434	1.1434	1.1065	1.0763	1.1120	1.0879	1.1087	1.0816	1.1125
24 O	-0.4609	-0.4609	-0.4703	-0.4777	-0.4674	-0.4880	-0.4681	-0.4739	-0.4961
25 O	-0.4737	-0.4737	-0.5005	-0.5695	-0.4986	-0.4795	-0.5000	-0.5311	-0.4828
26 N	-0.2928	-0.2928	-0.3133	-0.5415	-0.2958	-0.3140	-0.3055	-0.5182	-0.2932

Table 2. Calculated energies, dipole moment and frontier molecular orbital energies of compounds **T1**-**T9** from the B3LYP/6-311+G(d,p) basis set calculations.

Compounds	HOMO (eV)	LUMO (eV)	$\Delta E_{H\text{-}L}$ (eV)	Dipole (Debye)	E [B3LYP] (a.u.)
T1	-0.2439	-0.1118	-0.1321	4.879	-1574.555
T2	-0.2513	-0.1163	-0.1350	9.484	-1727.239
T3	-0.2424	-0.1114	-0.1310	6.676	-1916.415
T4	-0.2374	-0.1088	-0.1286	6.057	-1723.427
T5	-0.2432	-0.1118	-0.1314	6.5614	-1837.749
T6	-0.2430	-0.1144	-0.1286	7.129	-1952.270
T7	-0.2429	-0.1112	-0.1317	6.440	-1877.082
T8	-0.2294	-0.1095	-0.1199	7.1553	-2142.466
T9	-0.2445	-0.1131	-0.1314	6.8231	-1821.703

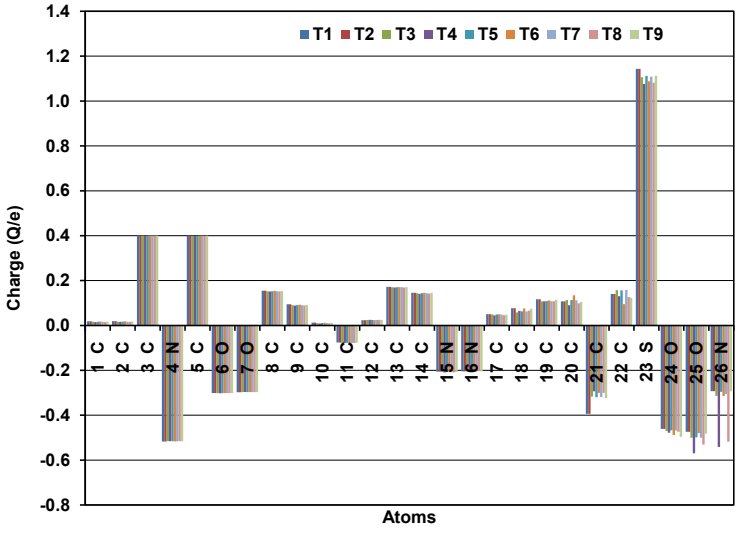

Figure 2. Graphical reorientations of Mulliken charge distributions of compounds **T1**-**T9**.

Furthermore, the orbital shapes (HOMO-LUMO) and the energy gap between the HOMO-LUMO which is a critical parameter to determine molecular electrical transport properties [27,28] were plotted in 3-dimensional (3D) by using at B3LYP/6-311+G(d,p) levels, respectively, are given in Figure 3. The values of the calculated energies, dipole moment and frontier molecular orbital energies of studied compounds (T1-T9) from the B3LYP/6-311+G(d,p) basis set calculations are given in Table 2. The lower value of dipole moment found 4.879 of compound **T1** and highest value 9.484 of compound **T2**. The higher values for HOMO energy level was -0.2513 of compound **T2**, also the lower values for LUMO energy level was -0.1088 of compound **T4**.

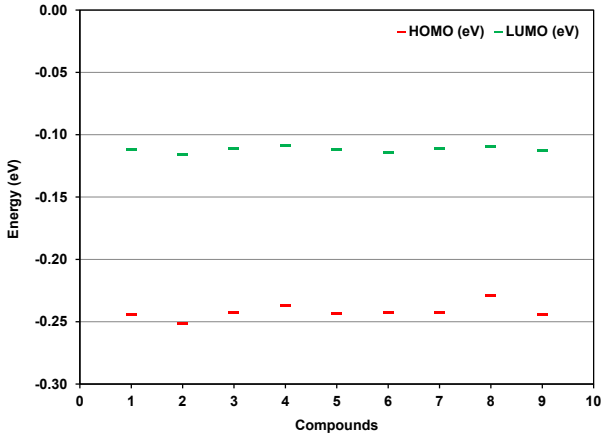

Figure 3. Frontier molecular orbitals and the energy gap between the HOMO-LUMO of compounds **T1**-**T9** by using at B3LYP/6-311+G(d,p) basis set calculations.

4. Conclusions

Nine new heterocyclic azo compounds were prepared by coupling the diazonium salts with *N*-(4-methylpheneyl) maleimide and different sulfa compounds and characterized. Density function theory at B3LYP level calculation was performed. HOMO-LUMO energies of the studied compounds was calculated by the 6-311+G(d,p) higher basis set level. Mulliken charge distributions of the investigated compounds were also computed at same level of method.

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Disclosure statement

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