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Research Article

Investigation of aromatic compounds to achieve the use of borazine part for the design of molecular dyes

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ABSTRACT

Aromatics form a wide group of compounds that include benzene and compounds that are similar to benzene in terms of chemical behavior. Unlike alkenes and alkynes, benzene and other aromatic compounds do not show a tendency to carry out addition reactions, in this research, aromatic compounds were investigated to achieve the use of the borazine part for the design of molecular dyes. After collecting the data, Hyper Chem 8.0.3 Gaussian Viewer, Chem Draw software were used to analyze the data. The results obtained from hyperpolarizability calculations showed that the magnitude of the first hyperpolarizability tensor of all molecules is relatively average, and NO_2 and NH_2 have the highest amounts of N and B isomers, respectively. Also, the calculations showed that the first hyperpolarizability value of the isomer is higher than the isomer B with the substitutions removed. On the other hand, these amounts of the N isomer are lower than the β isomer with donor substitutions.

Keywords: Aromatic, borazine, molecular dyes, polarizability

1. Introduction

Computational chemistry makes chemical phenomena possible without conducting experimental experiments. This method not only examines stable molecules, but also examines short-lived molecules, unstable intermediates, and even transition states, and in this way, it is possible to obtain information about molecules and reactions that it is impossible to check them experimentally. Aromatics form a wide group of compounds that include benzene and compounds that are similar to benzene in terms of chemical behavior. Some of these materials do not even look like benzene. Unlike alkenes and alkynes, benzene and other aromatic compounds do not show a tendency to perform addition reactions, but they participate in substitution reactions, which is one of the characteristic features of this class of substances. If functional groups are placed on the ring, they will affect the reactivity of the ring. The reactivity of the agents attached to the ring is also affected by the aromatic part [1]. Each carbon atom that belongs to the benzene ring contains two carbon-carbon sigma bonds, one carbon-hydrogen sigma bond and a double bond with the neighboring carbon atom in which the pi electron is decentralized. The bond order in all carbon-carbon bonds of this molecule is considered equal to 1.5 [2]. Due to potential applications in technologies such as lasers, telecommunications, photovoltaic cells, organic light emitting diodes and semiconductor layers in field effect transistors, information processing and holography, attention to materials with nonlinear optical properties (NLO) is increasing. Finds. Oligomers and polymers are an excellent alternative to traditional inorganic NLO crystals, as they can be easily synthesized and chemically modified. Very fast transfer time, resistance to high-intensity radiation, the possibility of making a thin layer and low electric power are important characteristics of NLO organic materials [3]. Borazine is a mineral compound consisting of boron, nitrogen and hydrogen elements. In this cyclic compound, three hydroborane units and three amino units are located in the middle. The structure of this compound is the same electron as benzene and for this reason it is called mineral benzene according to Nels Wiberg's proposal. This compound is also called Borazol, which comes from the German name of benzene, which is Benzol. Borazine is a colorless liquid with a special smell of aromatic compounds. This compound decomposes into boric acid, ammonia and hydrogen in water [4]. In 2018, Alipour et al investigated the nonlinear optical properties of two-dimensional MoS2 nanostructure. In this article, the nonlinear optical properties of the two-dimensional MoS2 nanostructure have been investigated using the Z-scan method by a continuous laser with different powers of 55 and 12 mW at a wavelength of 532 nm. Among these properties are the size and sign of the nonlinear refractive index and the nonlinear absorption coefficient, which were calculated with the help of Z-sweep test charts. Also, third-order non-linear acceptability was determined from 7-10 (esu) order. Such high third-order optical properties make this structure a suitable candidate for use in optoelectronic devices and phototransistors [5]. In 2018, Fusier reviewed the design of chromophores for photoinitiators of polymerization with a brief review and recent achievements. This review is devoted to an overview of chromophores that have been introduced over the past 50 years as photoinitiators of radical and cationic polymerization. Recent achievements for the design of light-sensitive compounds that are able to meet the challenge of working in media with low viscosity, with low light intensity in the visible wavelength range and under air [6]. In 2017, Marder investigated the design and synthesis of chromophores and polymers for electrooptic and photorefraction applications. The ability of nonlinear optical materials to transmit, process and store information forms the basis of emerging electronic and photonic technologies. Organic polymers containing chromophores, in which the refractive index is controlled by light or an electric field, are expected to play an important role [7]. Also, in 2015, Li et al. investigated polyurethanes containing indole-based nonlinear optical chromophores: from linear to H-type chromophores. Two new "H" types of indole-based chromophores were designed and successfully introduced into the polymer system, the resulting polymers show enhanced NLO effects, good processability, thermal stability, and almost excellent transparency [8]. , which shows the advantages of "H" type chromophore and they can be promising options for practical applications as new photonic materials. Since there has not been a study on aromatic compounds to achieve the use of the borazine part for the design of molecular dyes, and this research is considered a new research, therefore, in this research, aromatic compounds to achieve the use of the borazine part Borazine for the design of molecular dyes, investigating the effects of acceptor and donor substitutions (H, F, Cl, Br) (Me, NH_2, OH, COOH, CHO, CN, NO_2) on stability, dipole moment, polarization, frontal orbital, The structure, the most intense electron jump and hyperpolarizability were studied.

2. Experimental

From the point of view of the objective, the present research is one of the applied researches which has been carried out theoretically. In this study, in order to achieve the theoretical foundations of library studies, in which collection with tools such as: books, articles, sources, documents, archives, software, etc. will be used. After collecting the data, Hypertherm 8.0.3, Gaussian Viewer, Chem Draw software were used to analyze the data.

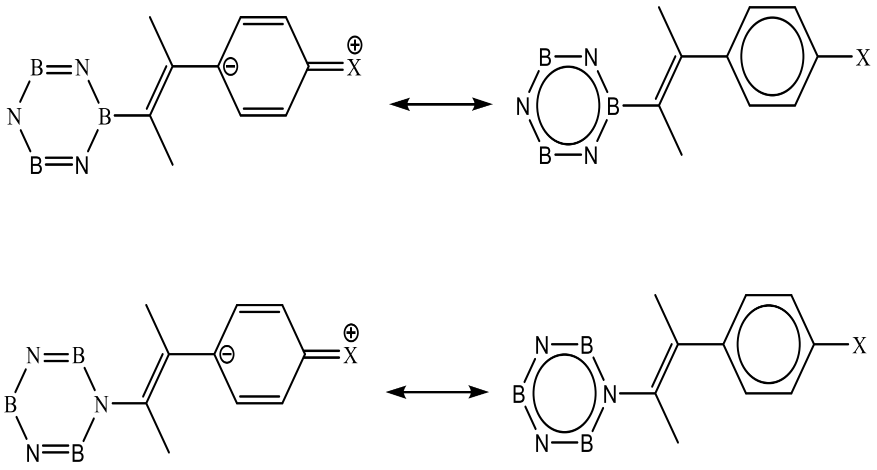
In any research, in order to obtain the best results, the choice of analysis tools and methods is very fundamental. In order to draw the structure of all molecules from the Hyperchem 8.0.3 software and in order to draw the desired structures to prepare the input files of the calculation software from Gaussian Viewer Version 3.07 and check the bond lengths and angles after the structures are optimized from the software Gaussian Viewer 3.07 is used. At the end, with the help of Chem Draw Version 9.0.1 software, the graphic drawing of all molecules was checked.

3. Results and discussion

In short, in this section, energetic aspects, dipole moment, polarizability, frontal orbital analysis, structural analysis, electron spectra and hyperpolarizability are discussed, as well as analysis with the help of Hyperchem software. Gaussian Viewer, Chem Draw done.

Energetic aspects

The investigation of benzene and dyes with borazine can be seen in Figure 1.



(I) (II)

Fig.1. Resonance form of dyes containing borazine with different x groups

Energy calculation, relative energies for all molecules can be seen in Table 1. The relative energy indicates that in all species, the B isomer is more stable than the N isomer.

Table 1. Absolute energy (Hartree), relative energy (ΔE), their Hammett constant (σp), dipole moment of dyes containing borazine with different x groups.

	E(N)	E(B)	ΔE	σ_p	μ_{tot}(N)	μ_{tot}(B)
H	-551.2612	-551.2867	16.0114	0.00	1.6170	1.1312
F	-650.5254	-650.5510	16.0681	0.15	1.5716	0.3888
Cl	-1010.883	-1010.9086	15.7131	0.24	2.0451	1.0524
Br	-3124.8041	-3124.8291	15.6812	0.23	1.9662	0.9264
OH	-626.5042	-626.5308	16.7007	-0.38	3.2086	2.2789
NH_2	-606.6340	-606.6614	17.1915	-0.57	3.8899	3.8318
Me	-590.5887	-590.6147	16.2763	-0.14	1.9659	1.7426
CN	-643.5280	-643.5516	14.8121	0.70	5.2518	4.3900
CF_3	-888.4017	-888.4258	15.1485	0.53	5.2419	2.4079
CHO	-664.6178	-664.6416	14.9093	-	4.3992	2.9788
COOH	-739.8939	-739.9179	15.1083	0.44	3.0916	1.5469
NO_2	-755.8200	-755.8431	14.4770	0.81	5.6899	4.6521

There is a good linear relationship between the values of relative energies along with their Hammett constant (σ_p) (19 (Figure 2)

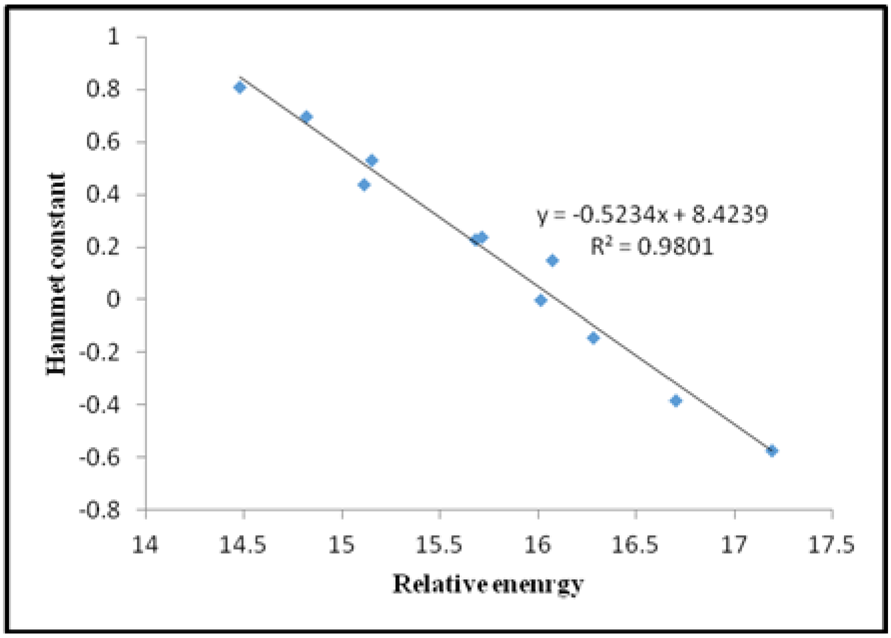
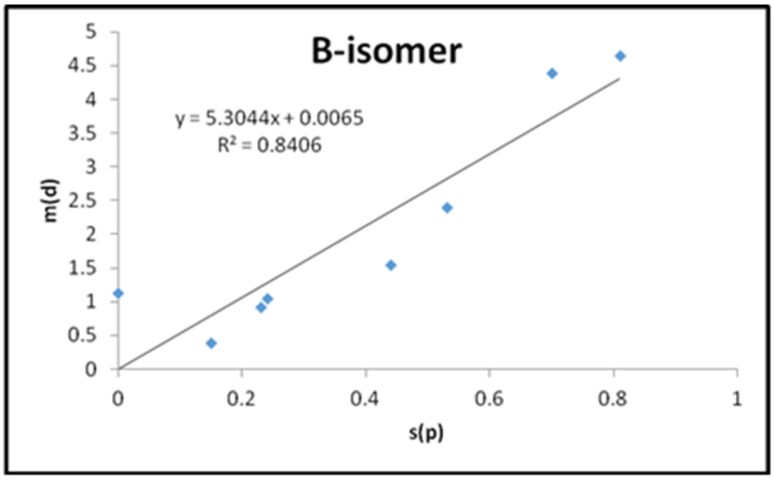


Fig.2. Relative energy relationship with their Hammett constant (σ_p)

Bipolar torque

The amount of N isomer has more dipole moment than B isomer. The relationship between and their Hammett constant (σ_p) can be seen in Figure 3.



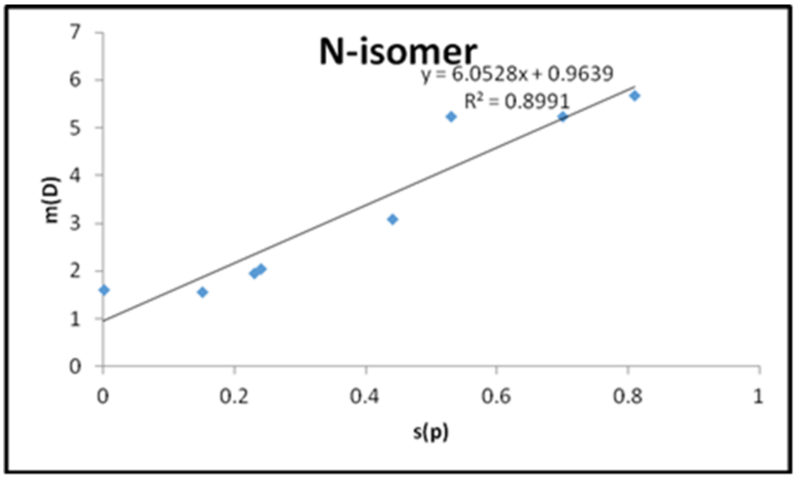


Fig.3. Dipole moment relationship with Hammett's constant (σp).

Polarizability

The reaction of a system in the applied electric field is described by polarizability, in addition to determining the strength of molecular interactions, it also determines the nonlinear optical properties of the system.

Using equation (1), isotropic polarization <α> is calculated as an average value:

$$\langle\alpha\rangle = \frac{(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})}{3} \quad (1)$$

And by using equation (2) the anisotropy polarizability is calculated as an average value:

$$\Delta\alpha = \left[\frac{(\alpha_{XX} - \alpha_{YY})^2 + (\alpha_{YY} - \alpha_{ZZ})^2 + (\alpha_{ZZ} - \alpha_{XX})^2}{2}\right]^{\frac{1}{2}} \quad (2)$$

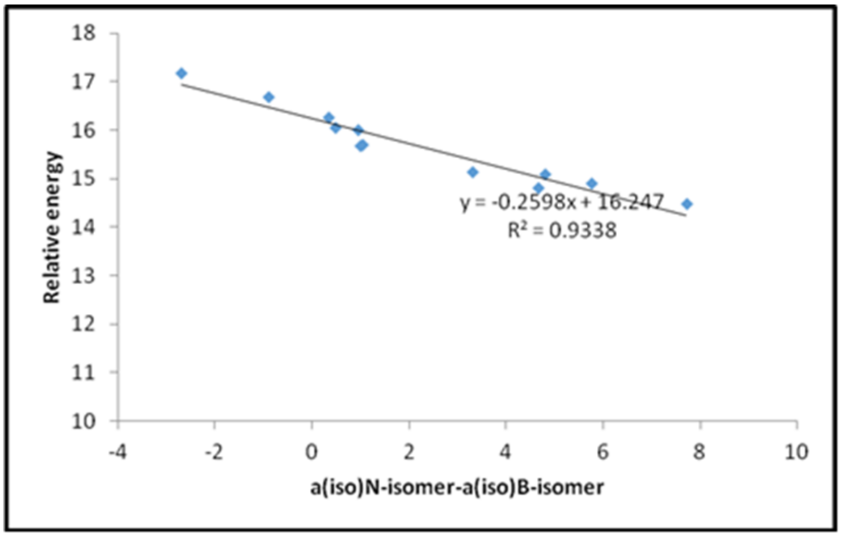
The results of calculating the amount of both isotropic and anisotropic polarization show the reduction of these values in stable complexes, as expected, using the principles of minimum energy and minimum polarizability in most cases except (OH, NH_2 = x) has been[9].

Table 2. isotropic and anisotropic polarization of dyes containing borazine with different x groups

	αxx	αyy	αzz	<α>	Δα
H	255.71	146.88	69.02	157.21	162.42
F	257.31	146.22	69.06	157.53	163.91
Cl	298.59	150.04	72.49	173.71	199.00
Br	314.96	153.43	75.96	181.45	211.20
OH	278.63	149.43	70.21	166.09	182.22
NH_2	304.09	152.91	72.38	176.47	203.75
ME	289.33	155.58	78.54	174.49	184.74
CN	317.68	150.19	75.19	181.03	215.03
CF3	278.75	153.74	79.25	170.59	174.61
CHO	310.82	158.57	74.32	181.24	207.62
COOH	312.53	160.04	75.68	182.75	207.93
NO_2	307.25	160.32	74.23	180.60	204.08

X	αxx	αyy	αzz	<α>	Δα
H	260.78	139.70	73.94	158.14	164.16
F	260.85	139.05	74.10	158.00	164.22
Cl	304.18	144.03	76.04	174.75	202.87
Br	320.34	147.51	79.45	182.44	215.10
OH	277.67	141.71	76.15	165.18	178.03
NH_2	297.11	144.44	79.75	173.77	193.31
ME	292.30	148.75	83.39	174.82	185.10
CN	335.43	147.45	74.20	185.70	233.39
CF3	292.31	150.50	78.86	173.90	188.15
CHO	331.83	155.85	73.32	187.01	228.70
COOH	330.59	156.57	75.49	187.56	225.76
NO_2	334.72	158.12	72.08	188.31	231.91

On the other hand, there is a good correlation between isotropic and anisotropic polarization values with relative energy values. (Figure 4)



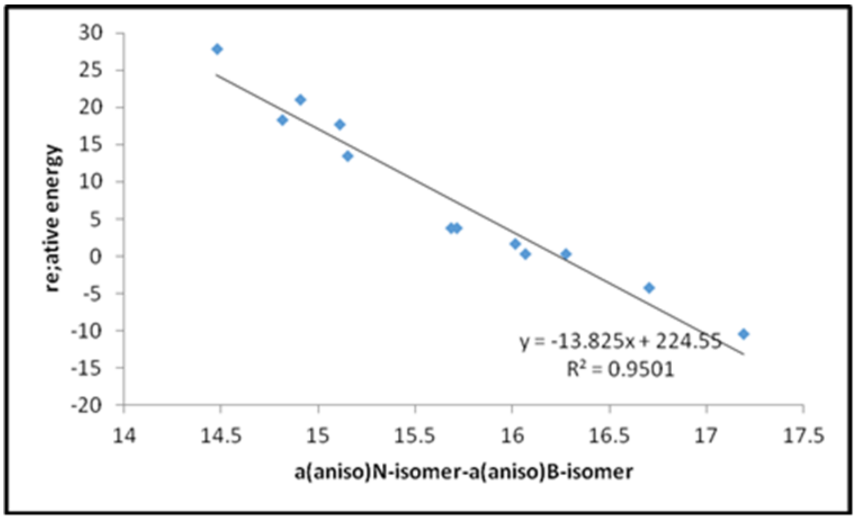


Fig.4. isotropic and anisotropic polarization relationship of α (iso)N-isomer-α (iso)B-isomer and α (aniso)N-isomer-α (aniso)B-isomer with Hammett constant (σp)

Frontal Orbital Analysis

The energy gap Eg between the highest occupied molecular orbital and the lowest empty molecular orbital is an interesting feature for these molecules. The energy gap is a reflection of the chemical activity of the molecule. In table 3, the frontal orbital energy values can be seen.

Table 3. frontal orbital energy (Hartree), gap energy (ΔE) and hardness (S) and chemical potential of dyes containing borazine with different x groups

	HOMO	LUMO	ΔE	η	S	μ	ω
H	-0.2307	-0.0586	4.6814	2.3407	0.2136	-3.9372	3.3113
F	-0.2316	-0.0606	4.6529	2.3264	0.2149	-3.9773	3.3999
Cl	-0.2345	-0.0670	4.5582	2.2791	0.2193	-4.1036	3.6944
Br	-0.2333	-0.0673	4.5193	2.2596	0.2212	-4.0909	3.7032
OH	-0.2158	-0.0514	4.4735	2.2367	0.2235	-3.6357	2.9548
NH_2	-0.2004	-0.0451	4.2273	2.1136	0.2365	-3.3414	2.6412
ME	-0.2242	-0.0553	4.5965	2.2982	0.2175	-3.8044	3.1488
CN	-0.2483	-0.0873	4.3799	2.1899	0.2283	-4.5666	4.7612
CF3	-0.2460	-0.0758	4.6327	2.3163	0.2158	-4.3801	4.1412
CHO	-0.2444	-0.0893	4.2194	2.1097	0.2369	-4.5416	4.8884
COOH	-0.2418	-0.0813	4.3685	2.1842	0.2289	-4.3973	4.4264
NO_2	-0.2545	-0.1051	4.0651	2.0325	0.2459	-4.8930	5.8895

	HOMO	LUMO	ΔE	η	S	μ	ω
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F	-0.2316	-0.0606	4.6529	2.3264	0.2149	-3.9773	3.3999
Cl	-0.2345	-0.0670	4.5582	2.2791	0.2193	-4.1036	3.6944
Br	-0.2333	-0.0673	4.5193	2.2596	0.2212	-4.0909	3.7032
OH	-0.2158	-0.0514	4.4735	2.2367	0.2235	-3.6357	2.9548
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CHO	-0.2444	-0.0893	4.2194	2.1097	0.2369	-4.5416	4.8884
COOH	-0.2418	-0.0813	4.3685	2.1842	0.2289	-4.3973	4.4264
NO_2	-0.2545	-0.1051	4.0651	2.0325	0.2459	-4.8930	5.8895

The obtained results show that the energy values of the highest occupied molecular orbital and the lowest empty molecular orbital decrease in molecular substitutions except (OH, NH_2, Me = x), and these values of the more stable diisomers also decrease. The linear relationship between frontier orbital energy and Hammett constant values can be seen in Figure 5.

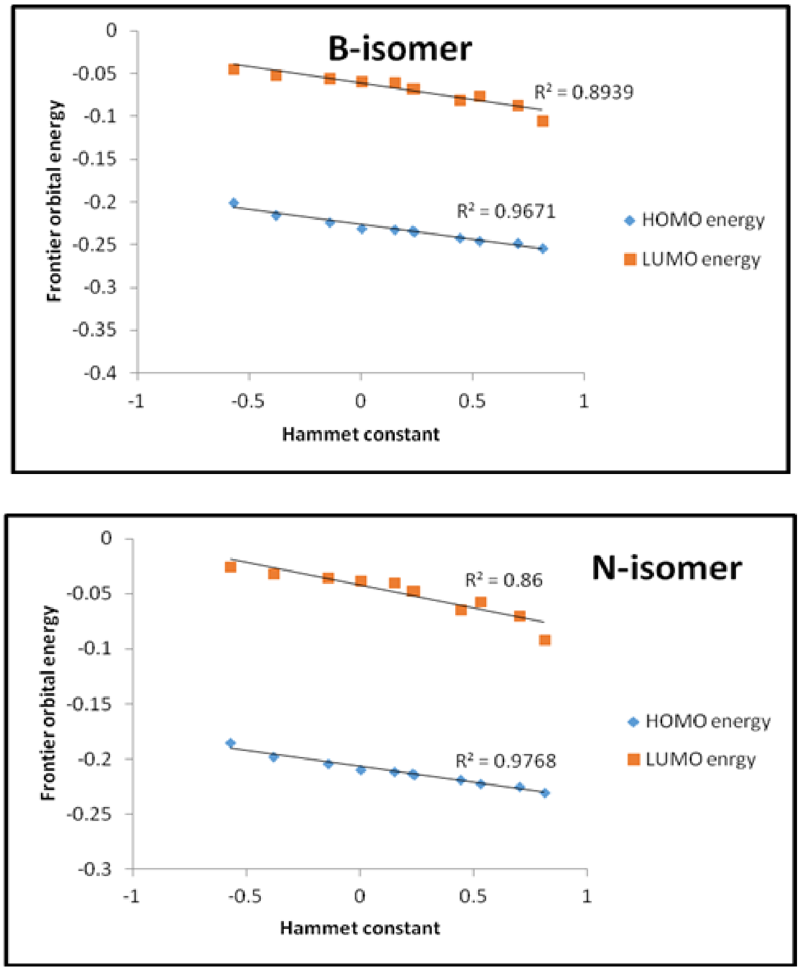

Fig. 5. Front orbital relationship with relative energy.

The energy gap of the highest occupied molecular orbital and the lowest empty molecular orbital of all structures can be seen in Table 3. These substitution values increase in the more stable isomer, as expected from the minimum and maximum hardness energy principles in most cases except (OH, NH2 = x) there is a good correlation between the relative hardness values and the constant values. (Figure 6)

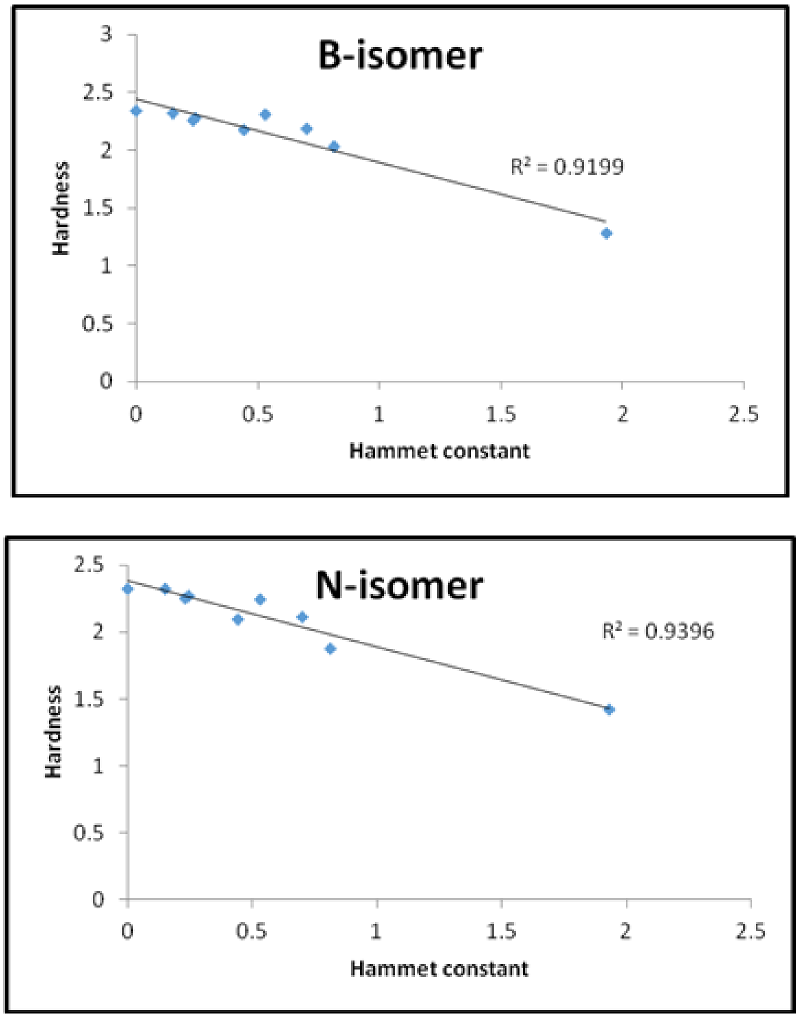

Fig. 6. Relationship between hardness values and Hammett's constant (except OH, Me, NH2)

To determine the chemical potential of these complexes, it can be obtained from the orbital energies of the highest occupied molecular orbital and the lowest empty molecular orbital using the following approximate expression:

$\mu=(\varepsilon HOMO + \varepsilon LUMO)/2$

These values indicate that the more stable isomer has a lower chemical potential .In order to determine the electrophilicity of these complexes, the □ index is calculated using the following expression [10]

$$\omega = \frac{\mu^2}{2\eta}$$

The electrophilicity index values in Table 3 show that the more stable isomer has the greatest electrophilicity.

Structural analysis

In Figure 1, the optimized geometry of the borazine-containing dyes studied in this research is shown by atom labeling. All the molecules that were investigated are essentially non-planar. Selected structural data for optimized structures with different x groups are presented in Table 4.

These values show that C1C2, C3C4, C5C6 bands are longer while B1N2 and B3N3 bands are shorter. These changes in band length indicate a greater contribution from the non-aromatic ion resonance structure.

Table 4. Maximum absorbed wavelength (λmax), oscillator strength of dyes containing borazine with different x groups

X	***B1 N1***	***N1B2***	***B2N2***	***N2B3***	***B3N3***	***N3B1***	***B1C2’***	***C1’C2’***	***C1’C1***	***C1C2***	***C2C3***	***C3C4***	***C4C5***	***C5C6***	***C6C1***
H	1.439	1.428	1.429	1.430	1.427	1.438	1.559	1.345	1.469	1.404	1.391	1.392	1.396	1.388	1.406
F	1.438	1.428	1.429	1.430	1.427	1.438	1.559	1.345	1.469	1.404	1.391	1.385	1.389	1.387	1.406
Cl	1.438	1.428	1.429	1.430	1.427	1.438	1.560	1.345	1.469	1.403	1.391	1.389	1.393	1.387	1.405
Br	1.438	1.428	1.429	1.430	1.427	1.438	1.560	1.345	1.469	1.403	1.391	1.390	1.394	1.388	1.405
OH	1.440	1.427	1.430	1.430	1.426	1.440	1.557	1.346	1.466	1.402	1.390	1.395	1.400	1.384	1.408
NH_2	1441	1.426	1.430	1.431	1.425	1.441	1.555	1.348	1.463	1.405	1.387	1.403	1.407	1.383	1.407
ME	1.439	1.427	1.429	1.430	1.426	1.439	1.558	1.346	1.468	1.402	1.392	1.396	1.403	1.386	1.406
CN	1.436	1.429	1.429	1.430	1.428	1.436	1.563	1.345	1.469	1.405	1.387	1.401	1.405	1.384	1.406
CF3	1.437	1.429	1.429	1.430	1.428	1.437	1.562	1.344	1.470	1.403	1.390	1.393	1.398	1.385	1.406
CHO	1.437	1.429	1.429	1.430	1.428	1.437	1.562	1.345	1.468	1.405	1.389	1.397	1.403	1.382	1.410
COOH	1.437	1.429	1.429	1.430	1.428	1.437	1.562	1.345	1.469	1.405	1.388	1.398	1.401	1.384	1.407
NO_2	1.436	1.480	1.429	1.430	1.429	1.436	1.564	1.345	1.469	1.406	1.388	1.390	1.393	1.388	1.407

N-isomer

X	N1 B1	B1N2	N2B2	B2N3	N3B3	B3N1	N1C2’	C1’C2’	C1’C1	C1C2	C2C3	C3C4	C4C5	C5C6	C6C1
H	1.445	1.424	1.428	1.429	1.425	1.447	1.417	1.340	1.468	1.405	1.391	1.393	1.395	1.389	1.406
F	1.445	1.424	1.428	1.429	1.425	1.447	1.417	1.340	1.468	1.405	1.391	1.385	1.388	1.389	1.406
Cl	1.446	1.423	1.428	1.429	1.424	1.448	1.415	1.341	1.466	1.405	1.390	1.389	1.392	1.388	1.406
Br	1.446	1.423	1.428	1.429	1.424	1.448	1.415	1.341	1.466	1.405	1.391	1.390	1.392	1.389	1.406
OH	1.444	1.425	1.428	1.428	1.426	1.446	1.420	1.340	1.467	1.403	1.391	1.394	1.398	1.386	1.408
NH_2	1.443	1.425	1.428	1.428	1.427	1.445	1.421	1.340	1.466	1.404	1.388	1.402	1.404	1.386	1.406
ME	1.444	1.425	1.428	1.429	1.425	1.446	1.418	1.340	1.467	1.402	1.392	1.396	1.402	1.387	1.407
CN	1.448	1.422	1.428	1.430	1.422	1.450	1.411	1.343	1.463	1.407	1.386	1.402	1.405	1.384	1.409
CF3	1.447	1.423	1.428	1.430	1.423	1.449	1.413	1.342	1.465	1.405	1.389	1.393	1.397	1.386	1.408
CHO	1.448	1.422	1.428	1.430	1.423	1.450	1.412	1.343	1.462	1.407	1.388	1.397	1.404	1.381	1.413
COOH	1.447	1.423	1.428	1.430	1.423	1.449	1.413	1.342	1.464	1.407	1.387	1.398	1.401	1.383	1.409
NO_2	1.449	1.422	1.428	1.430	1.422	1.451	1.410	1.343	1.462	1.409	1.386	1.391	1.394	1.384	1.410

Electron spectra

The most intense electron transfer (λmax) was obtained from the molecules. Table 5 shows the wavelength, oscillator resistance, composition of transitions obtained by TD-DFT calculations. These calculations show a decrease in λmax in the B isomer.

Table 5. Values of components β and β_{tot} (10-30 ecu) of dyes containing borazine with different x groups

		N-isomer		**B-isomer**	
	Character	**λ_{max}**	**f**	**λ_{max}**	**F**
H	HOMO→LUMO	286.95	0.6877	277.81	0.8117
F	HOMO→LUMO	288.60	0.5803	279.87	0.7579
Cl	HOMO→LUMO	294.37	0.7667	286.60	0.8986
Br	HOMO→LUMO	296.29	0.8082	290.02	0.9224
OH	HOMO→LUMO	296.39	0.5979	290.45	0.8057
NH_2	HOMO→LUMO	308.24	0.6218	306.66	0.8390
ME	HOMO→LUMO	290.82	0.7622	283.37	0.9175
CN	HOMO→LUMO	309.30	0.9708	295.71	0.9774
CF3	HOMO→LUMO	294.60	0.8166	281.36	0.8660
CHO	HOMO→LUMO	323.59	0.9312	306.52	0.9179
COOH	HOMO→LUMO	313.42	0.9459	298.05	0.9504
NO_2	HOMO→LUMO	352.16	0.6839	326.03	0.6617

There is a good correlation between σp and Δλmax (λmax N-isomer - λmax B-isomer) for all substitutions, except for Br and CN and Cl = x (Figure 7), the strongest electron transfer for all molecules to HOMO-LUMO transitions are attributed.

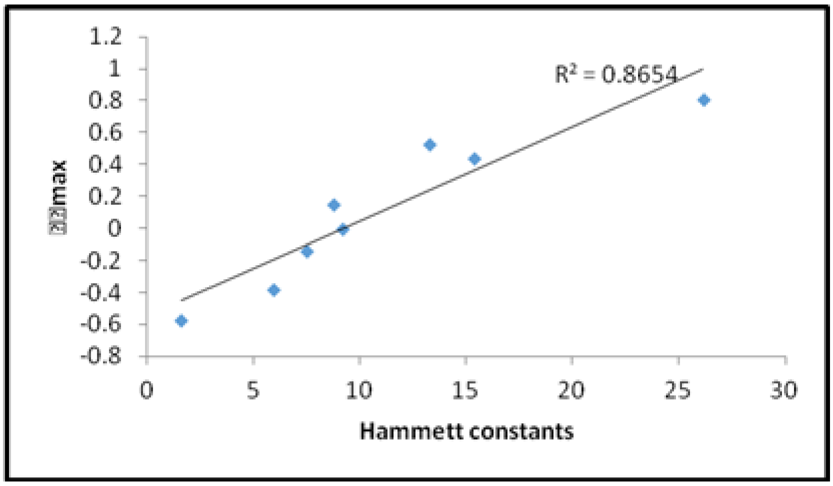

Fig. 7. Relationship between Δλmax (=λmax¬ N-isomer - λmax B-isomer) and Hammett constant (σp), except (Cl, CN, Br).

Hyperpolarizability

In Table 6, the first values of static Hyperpolarizability (βtot) can be seen for all molecules.

Table 6. β Components and βtot values (10-30 esu) for dyes containing borazine with different X- groups

X	H	F	Cl	Br	Me	NH_2	CN	COOH	CHO	NO_2	CF_3	OH
β_{XXX}	27.92	26.61	21.49	20.99	29.33	57.02	15.42	4.93	68.14	3.67	10.33	48.85
β_{XXY}	-9.91	-13.85	-11.08	-10.08	-33.26	-24.01	-6.88	-1.79	-25.08	-4.08	-7.31	-21.73
β_{XYY}	4.12	1.54	-0.66	0.10	10.95	7.76	-1.39	3.56	14.93	3.49	1.20	4.83
β_{YYY}	4.43	7.11	10.78	9.09	16.90	10.21	7.00	0.90	-5.81	3.09	3.94	3.26
β_{XXZ}	-42.46	-46.68	-19.80	-7.01	-63.98	-78.85	-6.25	20.84	-24.35	22.80	0.61	-65.60
β_{XYZ}	22.02	30.45	21.38	13.69	22.40	35.23	14.20	0.84	23.86	-1.27	14.17	39.39
β_{YYZ}	17.17	21.99	33.30	37.40	-13.14	32.28	43.58	47.38	30.67	47.21	41.22	24.84
β_{XZZ}	-73.27	-125.84	-127.38	-144.89	-119.27	-341.15	49.14	127.63	158.15	247.97	-0.65	-214.01
β_{YZZ}	44.32	74.29	86.67	94.46	76.66	298.37	-25.12	-83.97	-92.64	-156.04	-0.49	96.98
β_{ZZZ}	702.19	1222.74	1411.03	1642.97	1291.75	3344.65	-265.34	-959.81	-1360.79	-2515.21	192.77	2159.49
β_{tot}	5.87E-30	1.04E-29	1.24E-29	1.45E-29	1.05E-29	2.87E-29	2.06E-30	7.83E-30	1.19E-29	2.13E-29	2.03E-30	1.84E-29
$\beta_{tot}\times10^{-30}$	5.87	10.4	12.36	14.52	10.53	28.7	2.06	7.83	11.93	21.28	2.03	18.37

X	**H**	**F**	**Cl**	**Br**	**Me**	**NH_2**	**CN**	**COOH**	**CHO**	**NO_2**	**CF_3**	**OH**
β_{XXX}	247.31	-62.44	-70.46	-71.57	-72.78	-52.44	-78.01	-84.23	-28.74	-83.25	-73.97	-54.15
β_{XXY}	56.14	1.42	8.41	10.24	-10.93	0.55	19.91	25.08	1.05	23.13	18.90	-7.18
β_{XYY}	-118.15	6.78	-0.60	-1.83	14.06	10.16	-6.89	-4.92	5.59	-2.67	-7.83	9.90
β_{YYY}	10.69	1.80	9.41	11.30	14.80	10.00	4.63	1.12	-4.83	2.69	5.99	1.17
β_{XXZ}	-16.83	130.47	168.08	183.09	121.68	124.45	205.88	231.36	196.48	2.22	191.36	124.20
β_{XYZ}	55.60	32.42	15.30	6.60	15.46	46.48	-19.69	-35.69	-19.04	-47.56	-14.32	48.57
β_{YYZ}	-4.49	-3.04	16.05	20.13	-32.96	-17.82	33.65	33.20	21.67	41.72	31.66	-9.35
β_{XZZ}	-24.05	-10.19	13.26	10.97	-1.53	-104.13	152.54	207.31	219.93	324.39	81.17	-56.11
β_{YZZ}	1.08	10.43	-1.62	-0.20	1.07	172.54	-117.38	-169.26	-174.82	-266.02	-73.68	27.66
β_{ZZZ}	7.03	234.41	79.71	157.52	59.52	1848.99	-2007.88	-2856.46	-3397.78	-5040.28	-1030.40	979.37
β_{tot}	1.09E-30	3.18E-30	2.34E-30	3.17E-30	1.38E-30	1.70E-29	1.53E-29	2.25E-29	2.76E-29	4.33E-29	6.99E-30	9.50E-30
β_{tot} □10^{-30}	1.09	3.18	2.34	3.17	1.38	17.02	15.31	22.45	27.57	43.27	6.99	9.5

The results from the above tables showed that the magnitude of the first hyperpolarizability tensor of all molecules is relatively average, and NO_2 and NH_2 have the highest amounts of N and B isomers, respectively. On the other hand, these N isomer values are lower than the β isomer with donor substitutions. A good correlation between βtot and λmax in the N isomer is shown for all substitutions (Figure 8). But there is a similar relationship in isomer B for donor substitutions and removing substitutions.

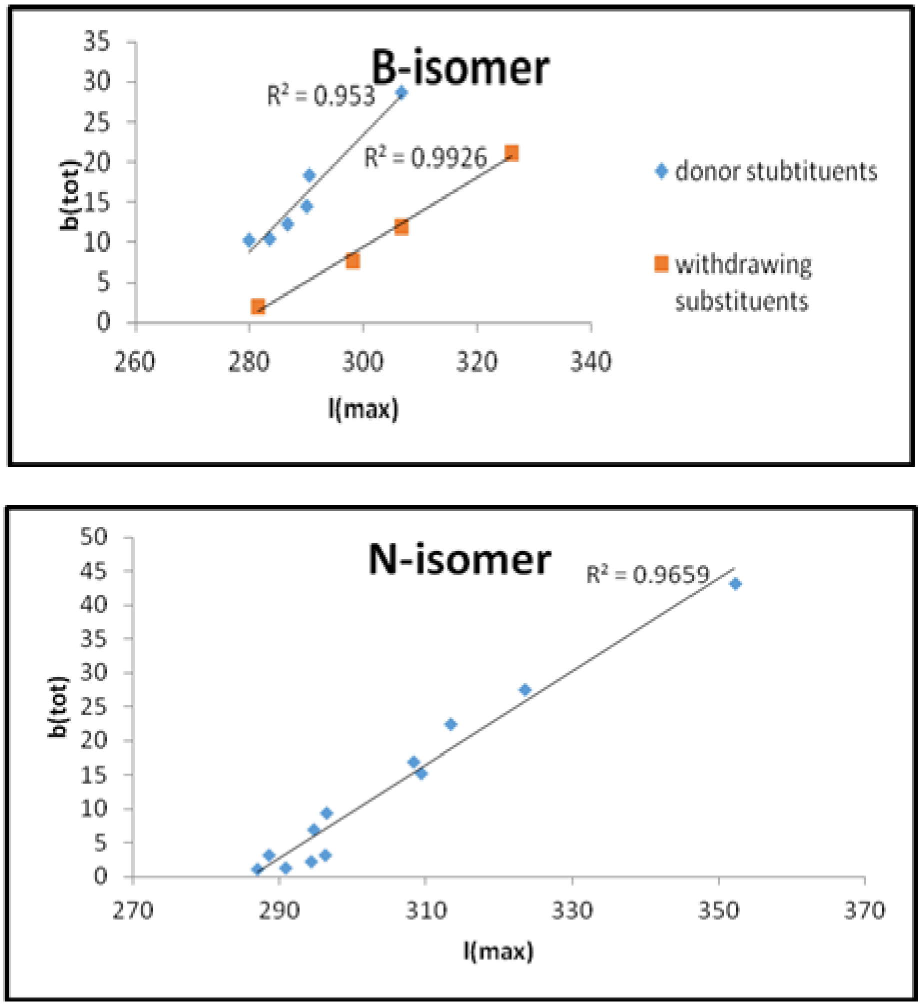

Fig. 8. The relationship between the first polarizability (βtot) and λmax

4. Conclusion

The study of electrical, structural, spectroscopic properties, as well as the first static hyperpolarizability of dyes with borazine showed that the stability of B isomer is higher than N type. The reduction of isotropic and anisotropic polarization values and the increase of HOMO-LUMO gap values in stable complexes were inconsistent with the principles of minimum energy and minimum polarization in most cases (except OH, NH_2 = x). Calculations showed that in all molecules, the most intense electron jump is due to HOMO-LUMO transition. The results of theoretical research showed that the substitutions of the acceptor (acceptor) lead to an increase in the values of the first hyperpolarizability in the N isomer compared to the B isomer. This amount is lower in the N isomer than in the B isomer with the substituent. The results of energy calculation showed that relative energy in all species, B isomer is more stable than N isomer. Also, the calculations revealed that the N isomer has more dipole moment than the B isomer. The results of calculating the amount of both isotropic and anisotropic polarization show the reduction of these values in stable complexes, as expected from the principles of minimum energy and minimum polarizability in most cases (except OH, NH_2 = x) the results obtained They show that the energy values of the highest occupied molecular orbital and the lowest empty molecular orbital in molecular substitutions except OH, NH_2, Me = x and also these values of the more stable diisomers decrease.

In the following, the optimized geometric shape of dyes with borazine has been studied (Figure 1). Also, selected structural data were calculated for the optimized structures, which show that C1C_2, C3C4, C5C6 bands are longer and B1N2 and B_3N_3 bands are shorter. These changes in the band length indicate that the majority contribution is from the non-aromatic ion resonance structure. The results obtained from the most intense electron transfer (λmax) of the molecules show the reduction of λmax in isomer B. For all substitutions, except for Br, CN and Cl = x, the strongest electron transfer for all molecules is attributed to HOMO-LUMO transitions. The results obtained from hyperpolarizability calculations showed that the magnitude of the first hyperpolarizability tensor of all molecules is relatively average, and NO_2 and NH_2 have the highest amounts of N and B isomers, respectively. Also, the first hyperpolarizability value of the isomer is higher than the B isomer with substitutions removed, and on the other hand, these N isomer values are lower than the β isomer with donor substitutions.

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