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Ab initio Hartree-Fock calculations on linear and second-order nonlinear optical properties of new acridine-benzothiazolylamine chromophores

Davut Avcı · Hüseyin Cömert · Yusuf Atalay

Abstract The calculation of optimized molecular structure and molecular hyperpolarizability of four new acridine-benzothiazolylamine chromophores (1–4) [2-nitro-6-(piperid-1-yl) acridine (1), 6-(benzothiazol-2-yl-amino)-2-nitro-acridine (2), 6-(6-ethylcarboxylate-benzothiazol-2-yl-amino)-2-nitroacridine (3), 6-(6-(β-hydroxyethyl-benzothiazol-2-yl-amino)-2-nitroacridine (4)] have been investigated using *ab initio* methods. *Ab initio* optimization were performed at the Hartree–Fock level using STO-3G basis set. The first hyperpolarizabilities have been calculated at the Hartree–Fock method with 6–31G and 6–311G basis sets using Gaussian 98W. In general, the first hyperpolarizability is dependent on the choice of method and basis set. To understand this phenomenon in the context of molecular orbital picture, we examined the frontier molecular orbital energies of all the molecules by using HF/6–31G, 6–311G levels. The polarizability, anisotropy of polarizability and ground state dipole moment of all the molecules have also been calculated. These acridine-benzothiazolylamine chromophores display significant second–order molecular nonlinearity, β (60.2–137.0×10^{-30} esu) and provide the basis for future design of efficient nonlinear optical materials having the acridine-benzothiazolylamine core.

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Introduction

Nonlinear optics (NLO) deals with the interactions of applied electromagnetic fields in various materials to generate new electromagnetic fields, altered in frequency, phase, or other physical properties. NLO materials have been attractive in recent years with respect to their future potential applications in the field of optoelectronic such as optical communication, optical computing, optical switching and dynamic image processing [1, 2]. Due to their high molecular hyperpolarizabilities, organic materials display a number of significant nonlinear optical properties. NLO materials were categorized as multilayered semi-conductor structures, molecular based macroscopic assemblies and traditional inorganic solids. A variety of inorganic, organic and organometallic molecular systems have been studied for NLO activity [1].

Experimental measurements and theoretical calculations on molecular hyperpolarizability β become one of the key factors in the second-order NLO materials design [3, 4]. Theoretical determination of hyperpolarizability is quite useful both in understanding the relationship between the molecular structure and nonlinear optical properties. It also provides a guideline to experimentalists for the design and synthesis of organic NLO materials given in Fig. 1 [5]. Nonlinearity in organic chromophores can be synthetically modulated by varying the composition or length of conjugated π-systems, and by evaluating the effects of various electron-donor and -acceptor groups.
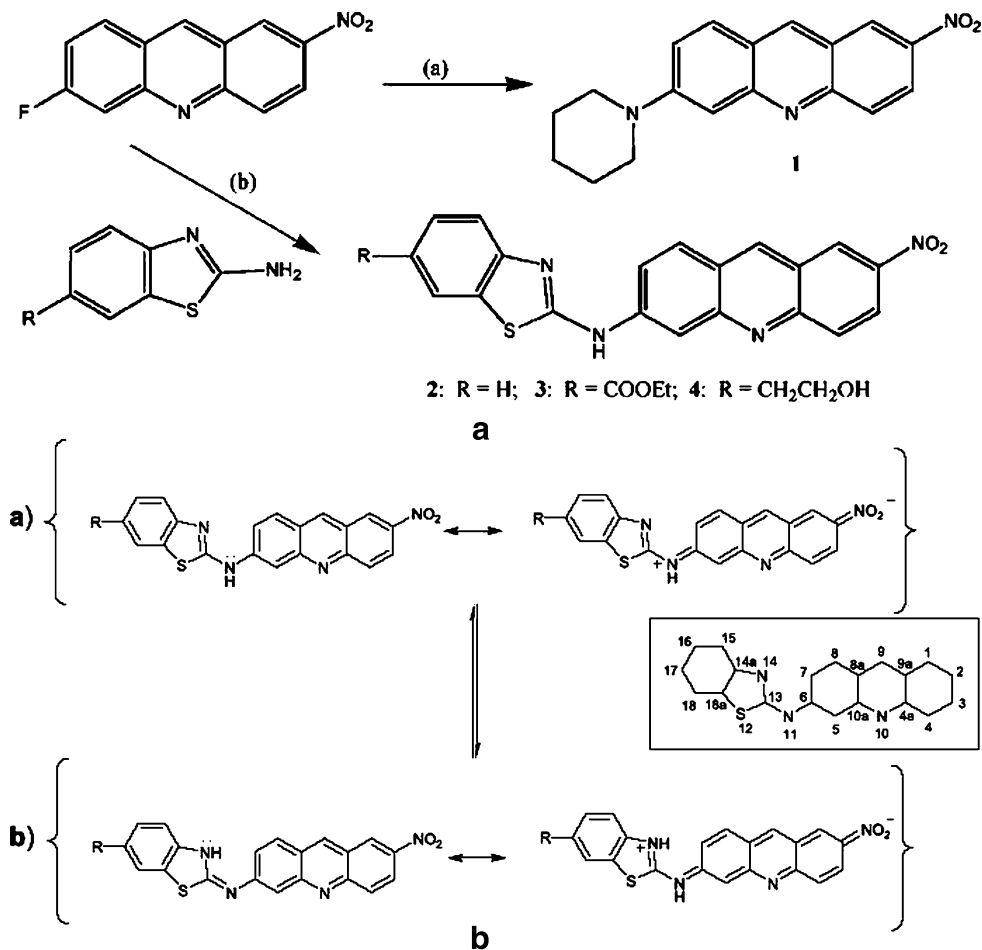
In previous work, new NLO motifs among acridine-based chromophores (1–4) [2-nitro-6-(piperid-1-yl) acridine (1), 6-(benzothiazol-2-yl-amino)-2-nitro-acridine (2), 6-(6-ethylcarboxylate-benzothiazol-2-yl-amino)-2-nitroacridine (3), 6-(6-(β-hydroxyethyl-benzothiazol-2-yl-amino)-2-nitroacridine (4)] were synthesized and characterized by ^{1}H NMR, ^{13}C NMR, IR and elemental analysis [5]. Also, vibrational spectra and GIAO ^{1}H NMR, ^{13}C NMR chemical shifts of these compounds were investigated by using *ab initio* Hartree-Fock method and density functional method (B3LYP) with 6-31G (d) basis set [6]. To the best of our knowledge, the theoretical calculations of first hyperpolarizability and the influence of variation highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbital energies on first hyperpolarizability for four new acridine-benzothiazolylamine chromophores (1–4) have not been investigated yet.

In this paper, theoretical calculations on ground state dipole moment, molecular polarizability, and molecular first hyper-polarizabiliy and frontier molecular orbital properties of these derivatives by using *ab initio* Hartree-Fock method with 6–31G, 6–311G basis sets have been investigated. Calculated first hyperpolarizability values were indirectly compared to the two state model static hyperpolarizability results.

Computational details

The first series of 1–4 were synthesized by Molinos-Gómez et al. (in Fig. 1) [5]. The geometry optimization of 1–4 was made using *ab initio* Hartree-Fock level with STO-3G minimal basis set. Optimized molecular structures of 1–4 are depicted in Fig. 2. The choice of a suitable basis set to calculate the NLO properties of 1–4 is important. The effects of basis sets on calculations of NLO properties are studied at the HF level with different basis sets, such as 6–31G, 6–311G, 6–31+G, 6–31G*, etc. However, the addition of polarization and diffuse functions for split and triple valence basis sets (6–31G, 6–311G, etc.) with calculations of NLO properties have greater computational cost. Thus, 6–31G and 6–311G basis sets appear to achieve the basis set limit for this work. All hyperpolarizability calculations of obtained optimized molecular structures of 1–4 have been carried out using *ab initio* Hartree-Fock method with 6–31G and 6–311G basis sets. Obtained first hyperpolarizability values using HF/6–31G, 6–311G levels are generally lower than the other basis sets. For example, for molecule 2, the value of β with HF/6–31+G has been calculated at 150.3×10^{-30} esu.

Fig. 1 (a) Synthetic sequences for new acridine-benzothiazolylamine obtained by A. Molinos-Gömez et al. [5]. (b) Tautomeric benzothiazol-2-yl-(7-nitroacridin-3-yl)amine (a) and (3H-benzothiazol-2-ylidene)-(7-nitroacridin-3-yl) amine (b) and their respective mesomeric forms [5]
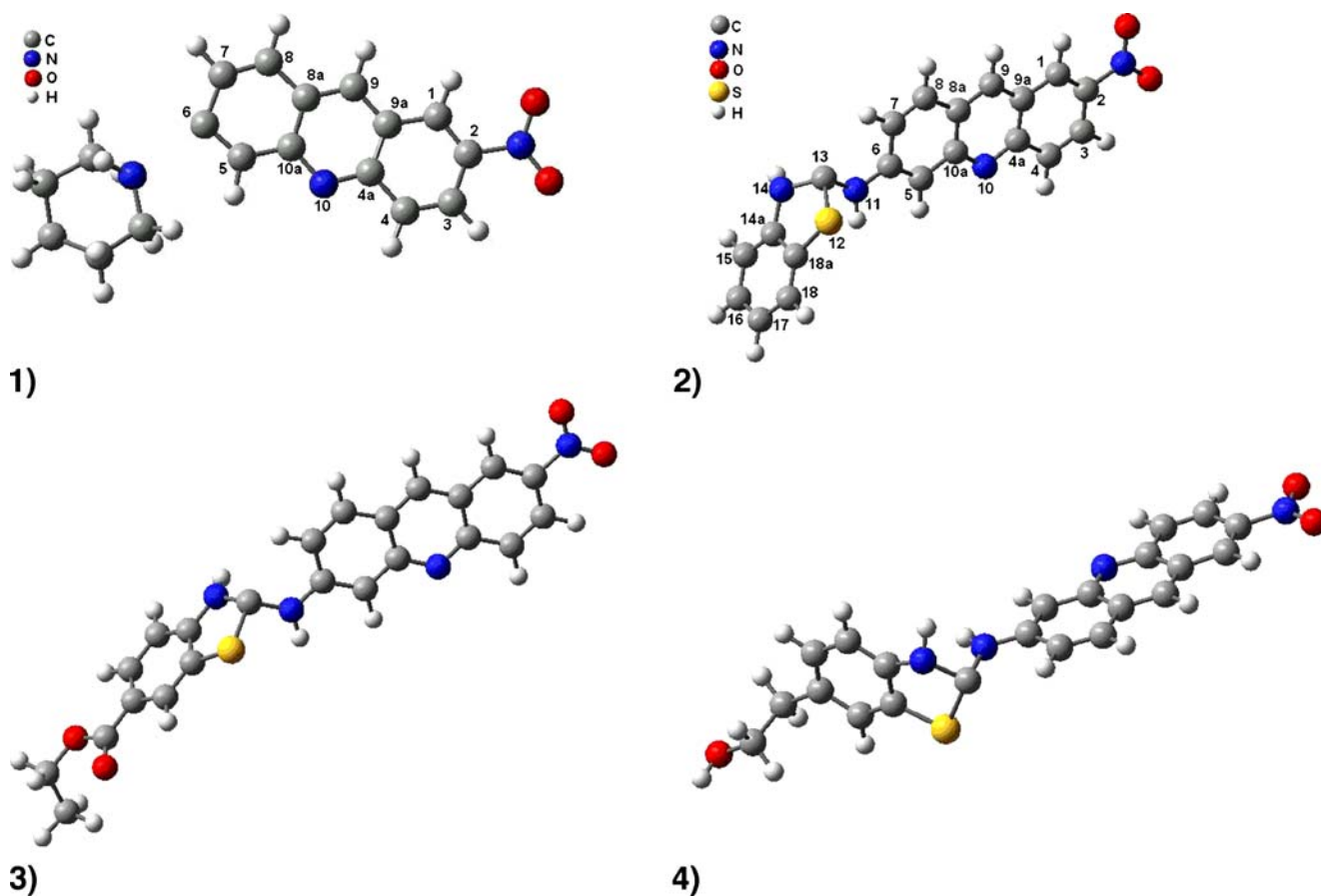
Fig. 2 Optimized molecular structure of 2-nitro-6-(piperid-1-yl) acridine (**1**), 6-(benzothiazol-2-yl-amino)-2-nitro-acridine (**2**), 6-(6-ethylcarboxylate-benzothiazol-2-yl-amino)-2-nitroacridine (**3**) and 6- (6-(β-hydroxyethyl-benzothiazol-2-yl-amino)-2-nitroacridine (**4**) by using HF/STO-3G level

The general quantum chemical approaches for molecular first hyperpolarizability β include sum-over-state (SOS) approach [7, 8], the finite-field (FF) approach [9], couple-perturbation Hartree-Fock (CPHF) approach [10], etc.

The static quadratic polarizability (β) in the two-state model of Kanis et al., Oudar and Chemla [1, 7, 8] has been calculated using Eq. (1) that differs from other conventions [11] by appropriate numerical factors. In this model, β implies that frequency doubling will be enhanced near resonance either of the single photon or the two photon type, or by increasing the "allowedness" or charge-transfer character of the important transition

$$\beta \propto \left(\mu_{ee} - \mu_{gg}\right)\frac{\mu_{ge}^2}{E_{ge}^2}. \tag{1}$$

In this configuration $\Delta\mu = \mu_{ee} - \mu_{gg}$ denotes the change of the dipole moments from the charge transfer excited state to the ground state. μ_{ge} and E_{ge} are transition dipole moment and excited energy from the ground state to the charge-transfer excited state.

Three different treatments are often used for the static first hyperpolarizability from individual tensor elements in the literature denoted as β_{vec}, $\beta_{\parallel}$ and β. A measurement of the second-order polarizability β_{vec} is related to second-harmonic generation (SHG). Although all 27 components of the β tensor can be computed, only the vector component along the dipole moment direction (β_{vec}) is sampled experimentally in electric field induced second-harmonic generation (EFISH) experiments. Thus, the β_{vec} is defined as [1, 12, 13]:

$$\beta_{vec} = \sum_{i=1}^{3}\frac{\mu_i\beta_i}{|\mu|}. \tag{2}$$

Here, μ is ground-state molecular dipole moment and

$$\beta_i = \beta_{iii} + \frac{1}{3}\sum_{j\neq 1}\left(\beta_{ijj} + \beta_{jij} + \beta_{jji}\right)$$

where i and j run over the molecular cartesian directions x, y, and z. In chromophores where the charge-transfer direction is obviously parallel with the ground-state dipole

moment direction (for purposes of illustration, the x direction), some authors label their experimental or theoretical responses as β_x or β_{xxx}. There is another quantity of interest in this study, the total hyperpolarizability (intrinsic quadratic hyperpolarizability), β_{tot}

$$\beta_{tot} = \left(\beta_x^2 + \beta_y^2 + \beta_z^2 \right)^{1/2} \qquad (3)$$

β_{vec} will be identical to β_{tot} when the charge transfer is unidirectional and parallel to the molecular dipole moment. Note that β_{tot} is always a positive quantity regardless of the sign of the individual vectorial components and measured using hyper Rayleigh scattering (HRS) experiment. Since β values of Gaussian 98 W output are in atomic units (a.u.), they have been converted into electronic units (esu) (1 a.u. = 8.6393×10^{-33} esu).

The mean polarizability (α) and anisotropy of polarizability ($\Delta\alpha$) of these molecular systems can be calculated using the following equations.

$$\langle\alpha\rangle = 1/3\left(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}\right) \qquad (4)$$

$$\Delta\alpha = 1/2\left[\left(\alpha_{xx} + \alpha_{yy}\right)^2 + \left(\alpha_{yy} + \alpha_{zz}\right)^2 + \left(\alpha_{zz} + \alpha_{xx}\right)^2\right]^{1/2}. \qquad (5)$$

All calculations are carried out by using Gaussian 98 W program package [14] and Gauss-View molecular visualisation program [15].

Experimental first static hyperpolarizability (two-state model) values cannot be directly compared to our theoretical results, but to the general trend. Herein, due to the lack of calculated dipole moments of the excited states, the two-level Eq. (1) shown above could not be applied, and so the discussions were only limited to the qualitative level using Eqs. 2, 3, 4 and 5.

Results and discussion

We have fulfilled the polarizability, anisotropy of polarizability, first hyperpolarizablity and HOMO-LUMO energy gap of all the molecules at their respective most stable geometries using *ab initio* method HF level with STO-3G basis set. From the computed tensorial components β_{total} and β_{vec} are calculated for respective molecules by taking into account the Kleinman symmetry relations and the squared norm of the cartesian expression for the tensor β [16]. The relevant expressions used for the calculation are as shown above Eq. (3). All the polarizability and hyperpolarizability components values were calculated using Gaussian 98 W (α_{xx}, α_{xy}, α_{yy}, α_{xz}, α_{yz}, α_{zz} and β_{xxx}, β_{xxy}, β_{xyy}, β_{yyy}, β_{xxz}, β_{xyz}, β_{yyz}, β_{xzz}, β_{yzz}, β_{zzz}) for the molecular systems. The first hyperpolarizability, mean polarizability and anisotropy of polarizability values are calculated using above Eqs. (3), (4) and (5). All the polarizability (α) values and hyperpolarizability (β) values calculated using Gaussian 98 W for the molecular systems are given in Tables 1 and 2. Theoretical results of β for all the molecular systems can be indirectly compared to the two state model results.

Chromophores **2**, **3**, and **4** should behave similarly to **1** because the electronic distributions of the push–pull systems should themselves be similar. Alternatively, slightly lower intensities could be observed for **2**, **3**, and **4** as compared to **1**, which would be consistent with the findings of Moylan for dialkyl-diarylamino derivatives [5]. Surprisingly the NLO responses of **2**, **3**, and **4** were all greater than that of **1** by nearly 50%. This difference can be caused by the existence of minor tautomeric forms capable of acquiring a stabilized, highly polarized charge-transfer state. First and static hyperpolarizability (β,β_0) results are shown in Table 3. In molecule **1**, a considerable decrease in comparison with β at 1064 nm was observed, in which the $\beta(0)$ was 20% lower than that of the reference compound DANS [5]. However, first hyperpolarizability value for molecule **1** has been calculated at 60.2×10^{-30} esu, 57.3×10^{-30} esu (HF/6–31G,

Table 1 All α components (in a.u.) and average value ($<\alpha>$, in a.u.) calculated using *ab initio* Hartree-Fock method with 6–31G and 6–311G basis sets for all molecular systems shown in Fig. 2

Molecule	α_{xx}	α_{xy}	α_{yy}	α_{xz}	α_{yz}	α_{zz}	$<\alpha>$
1[a]	282.5355145	0.2381969	97.8973296	95.1364163	-1.9774087	345.776875	242.07
1[b]	291.6081053	0.2389	113.3097612	95.6183862	-1.852427	354.8918641	253.27
2[a]	383.831756	6.50713	140.1577699	201.3403849	13.8576558	415.7859422	313.26
2[b]	393.6779563	7.2243719	158.8359629	200.0925998	13.1757823	428.9561146	327.16
3[a]	435.2149906	33.655318	195.3103283	216.6138119	25.4510728	445.8677814	358.80
3[b]	483.3975278	25.6420948	203.584039	154.3795224	-5.8845508	401.1399162	362.71
4[a]	415.9450269	-2.0194902	157.4198168	212.1545063	-5.947618	446.9832818	340.12
4[b]	465.1046975	-11.0905787	176.3687376	166.2431504	-11.1152733	405.5577549	349.01

Average polarizability ($<\alpha>$) are obtained from Eq. (4) and [a],[b] represent HF method with 6–31G and 6–311G basis sets calculations, respectively.

Table 2 First hyperpolarizability (all β components, in a.u. and β_{tot} value, in 10^{-30} esu) of four new acridine-benzothiazolylamine chromophores (1–4)

Molecule	Theoretical										
	β_{xxx}	β_{xxy}	β_{xyy}	β_{yyy}	β_{xxz}	β_{xyz}	β_{yyz}	β_{xzz}	β_{yzz}	β_{zzz}	β
1[a]	1559.7162107	29.3207042	-21.6354944	43.1277614	2453.3691673	-3.2235109	25.431092	3149.9022102	-14.5038736	2682.036666	60.2
1[b]	1442.6151669	37.5718 809	-57.4022074	60.7775187	2377.9788967	5.0607891	2.3065264	3075.8266658	-2.7287947	2532.7939444	57.3
2[a]	4996.0812291	-126.9184045	-150.1259178	-103.888825	5796.5487509	-92.9106711	-145.8578371	5900.5920622	-58.5901703	4869.7121648	129.9
2[b]	4771.8674846	-170.8524858	-174.3166362	-37.98819019	5594.0927805	-134.4877709	-179.0441599	5648.3296639	-99.0871015	4708.0931836	124.4
3[a]	3354.4944384	-1008.8829448	-952.0382666	-562.9803074	4189.6537125	-701.8149764	-695.5333031	4299.4237766	-497.3960529	3272.4842972	84.2
3[b]	4721.2996847	-874.3875261	-505.5532401	-89.5868909	6164.3448808	-123.7677081	-131.1511668	5690.3483138	-10.5836918	4087.3198375	122.6
4[a]	4139.828496	-180.4316113	-128.1005172	-62.0655632	4855.6335392	-150.6294942	-114.3579305	4817.6074131	-87.2323267	3586.2589924	104.8
4[b]	5790.8453255	-216.4181538	-90.1733585	36.7456915	6491.1681172	-175.8524354	-94.2487088	5977.923555	-95.2024643	4335.0112823	137.0

[a,b] represent HF method with 6–31G and 6–311G basis sets calculations, respectively, and β values are obtained from Eq. (3).

Table 3 Ground state dipole moment (μ, in D), average polarizability and anisotropy of polarizability ($<\alpha>$, $\Delta\alpha$, in a.u.), vector component of first hyperpolarizability and first static hyperpolarizability (β_{vec}, β_o, in 10^{-30} esu), and first hyperpolarizability (β, in 10^{-30} esu) values calculated using ab initio Hartree-Fock method with 6–31G and 6–311G basis sets for all molecular systems shown in Fig. 2

Molecule	μ	$<\alpha>$	$\Delta\alpha$	β_{vec}	β	β_o
1[a]	1.7810	242.07	157.74	44.7	60.2	43
1[b]	1.7731	253.27	153.43	49.6	57.3	43
2[a]	4.0097	313.26	184.64	-0.9	129.9	78
2[b]	4.2887	327.16	179.83	-2.6	124.4	78
3[a]	4.7995	358.80	173.53	-11.2	84.2	93
3[b]	5.6312	362.71	176.13	-14.3	122.6	93
4[a]	2.8325	340.12	194.71	21.3	104.8	-
4[b]	3.2065	349.01	186.71	29.8	137.0	-

Static hyperpolarizability (β_o) was calculated using the two state model taken from [5] and [a,b] represent HF method with 6–31G and 6–311G basis sets calculations, respectively.

6–311G levels), it was observed to be 43×10^{-30} esu. Similar values were not observed for the other chromophores. Chromophores **2**, **3** and **4** had β, β_0 values of 129.9×10^{-30} esu, 124.4×10^{-30} esu (for HF/6–31G and 6–311G levels), and 78×10^{-30} esu [5] and 84.2×10^{-30} esu, 122.6×10^{-30} esu (for HF/6–31G and 6–311G levels), and 93×10^{-30} esu [5], and 104.8×10^{-30} esu, 137.0×10^{-30} esu (for HF/6–31G and 6–311G levels), respectively. The larger value observed for **3** is probably due to an additional favourable effect on the tautomeric equilibrium stemming from the carboxylate group at the position **6**. Similar tensor components values were obtained for **2**, **3** and **4**, indicating that, most likely, the nonlinear polarizabilities of all of them are similar. The second order optical behaviours of **2**, **3**, and **4**, exhibited marked differences as compared to that of **1**, for which the second harmonic generation was clearly inferior. Considering that in all cases the electron-donor group directly linked to the 2-nitroacridine moiety is an amine, the variation in response must be attributed to the presence or absence of the benzothiazole. As the benzothiazole system is slightly π-deficient, the 2-aminobenzothiazole group of chromophores **2**, **3**, and **4** was expected to have a lower electron donating character than the piperidine present in **1** and, consequently, a lower NLO response. Surprisingly, calculated first hyperpolarizability values were the opposite. This state may be explained by the existence of tautomeric forms of the 2-aminobenzothiazole moiety (Fig. 2).

It is known that the magnitude of the polarizability and the first static hyperpolarizability of push–pull molecular systems are dependent on the efficiency of electronic communication between donor and acceptor groups as that will be the key to intra molecular charge transfer [17]. Charge-transfer bands in the UV-absorption spectra of **2**, **3**

Fig. 3 Frontier orbitals, LUMO at the right, HOMO at the left of the chromophores **1–4**

HOMO-(1)

LUMO-(1)

HOMO-(2)

LUMO-(2)

HOMO-(3)

LUMO-(3)

HOMO-(4)

LUMO-(4)
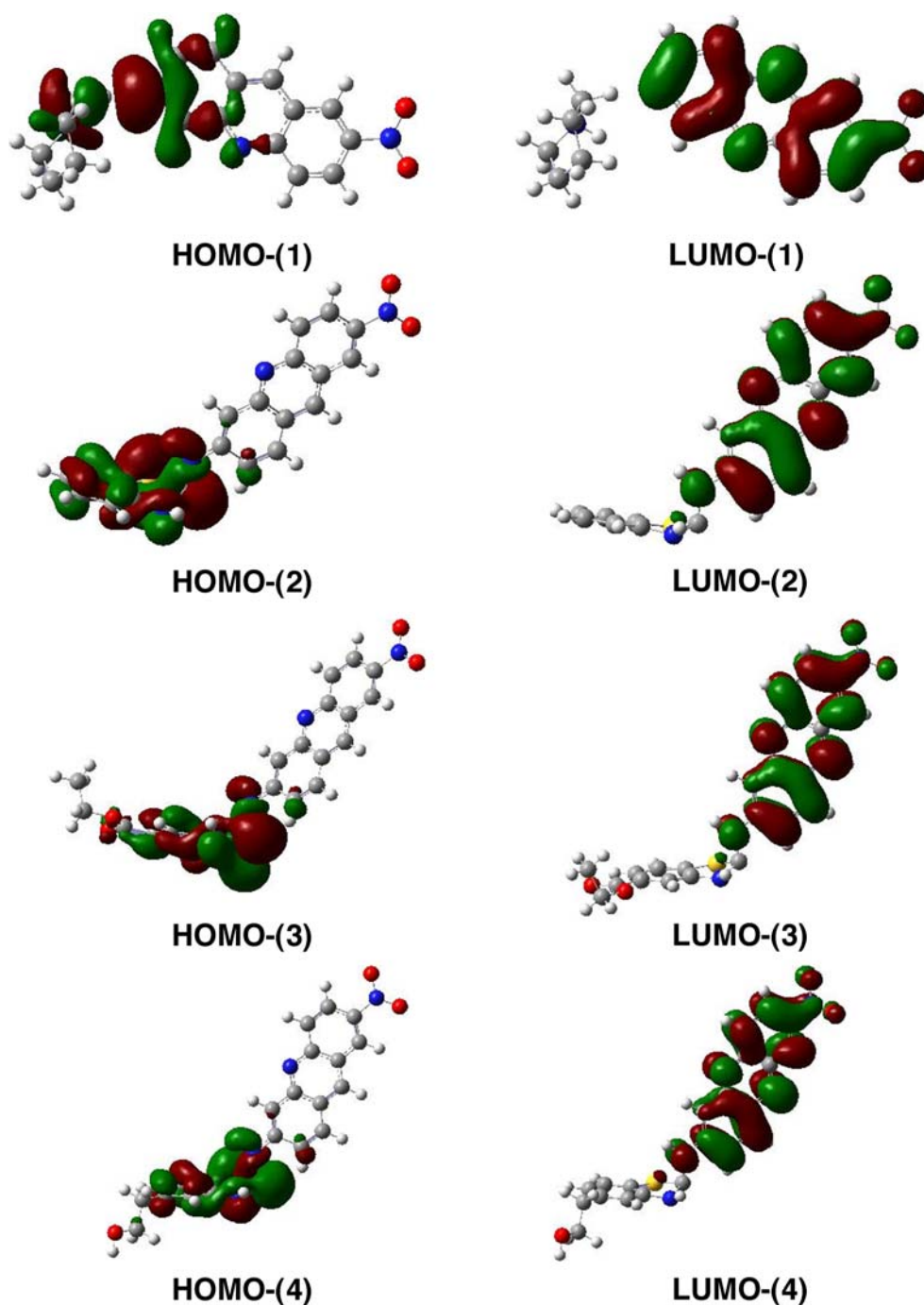
and **4** exhibit a hypsochromic displacement, whereas those of the spectra of **1** do not [5, 18]. This phenomenon suggested the presence of major aromatic tautomers, in which the slightly electron-deficient benzothiazole ring reduces the charge-transfer strength of the amino group [5]. To understand this phenomenon in the context of a molecular orbital picture, we examined the molecular HOMOs (the π_{donor}) and molecular LUMOs (the $\pi_{acceptor}$) generated via Gaussian 98 W. The HF/6–31G, 6–311G generated highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals of 1–4 are outlined in Fig. 3. The results for **1–4** are shown in Table 4. Figure 4

Table 4 HOMO-LUMO energy using HF/6–31G, 6–311G levels for all molecular systems shown in Fig. 2

Molecule	HOMO (a.u)	LUMO (a.u)	HOMO-LUMO energy gap (a.u.)
1[a]	-0.15151	0.10959	0.2611
1[b]	-0.15961	0.10466	0.26427
2[a]	-0.14123	0.09500	0.23623
2[b]	-0.14829	0.09102	0.23931
3[a]	-0.15187	0.09164	0.24351
3[b]	-0.15855	0.08775	0.2463
4[a]	-0.14347	0.09417	0.23764
4[b]	-0.14995	0.09031	0.24026

[a,b] represent HF method with 6–31G and 6–311G basis sets calculations, respectively.

shows the variation of HOMO-LUMO difference for **1–4**. It can be seen that there is an overlap between the molecular HOMO and LUMO which is necessary for obtaining large second order responses [1]. This situation can be clearly seen in Fig. 3. Besides, when Figs. 4 and 5 are investigated together, this overlap can be recognized. However, the benzothiazole system shows if slightly π-deficient, considerably increased the energy of the HOMO-LUMO energy gap for molecule **1** relative to **2**, **3** and **4**. Thus, the energy gap decreases with the substitution of the different electron-withdrawing groups (-COOEt, -CH$_2$CH$_2$OH) are indicated a larger hyperpolarizability. From here, the molecule **2** has the smallest energy gap and the largest β value which is presented in Table 2 and in Figs. 4 and 5. Figure 5 shows

the variation of hyperpolarizability of **1–4** and they clearly show the inverse relationship with HOMO-LUMO energy gap as shown in Fig. 4.

Also, in chromophores **2**, **3** and **4**, the polarizability increases with increasing substitution. Figure 6 shows the variation of polarizability and anisotropy of polarizability of **1–4**. Although chromophores **1**, **2**, **3** and **4** nearly show the parallel relationship with the hyperpolarizability as shown in Fig. 5, they clearly show the inverse relationship with HOMO-LUMO energy gap as shown in Fig. 4. In addition, ground state dipole moments of chromophores **1–4** have been calculated at 1.7731–5.6312 D range. These variations of dipole moment are listed in Table 3. Herein, the largest variations of dipole moment, the largest vector component of first hyperpolarizability and first hyperpolarizability have been calculated for molecules **3,1** and **2**, respectively.

Conclusions

The first hyperpolarizability is strongly dependent on the extent of the electronic communication between the donor group and the acceptor group through the bridge. In this study, the linear and nonlinear optical properties of molecules with the benzothiazol-2-yl-amino electron-donating group are considerably enhanced in relation to the analogous piperidyl compound. This phenomena is due to the contribution of a minor nonaromatic tautomer. These tautomers, previously described in the literature, have a less

**Fig. 4** Variation of HOMO-LUMO energy difference of molecule **1–4**
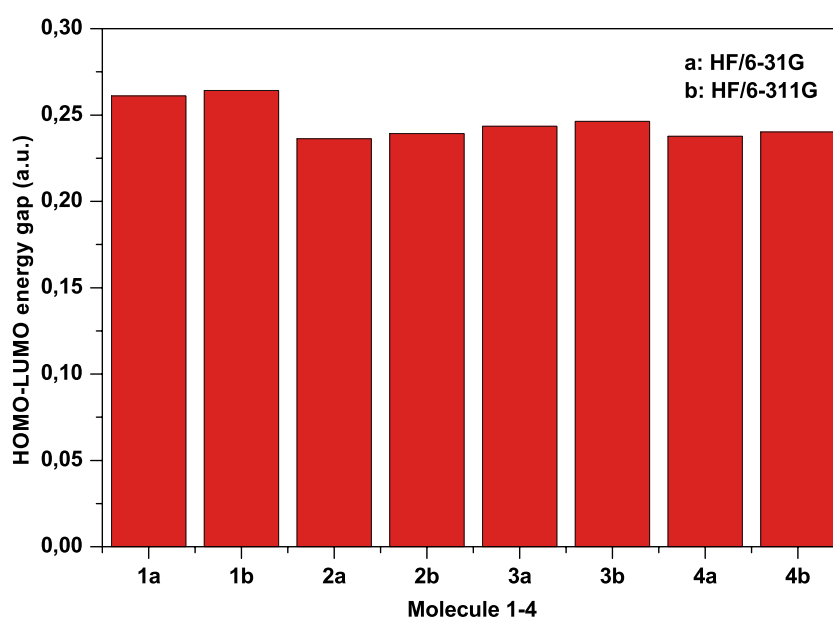
Fig. 5 Variation of theoretical hyperpolarizability of molecule **1–4**
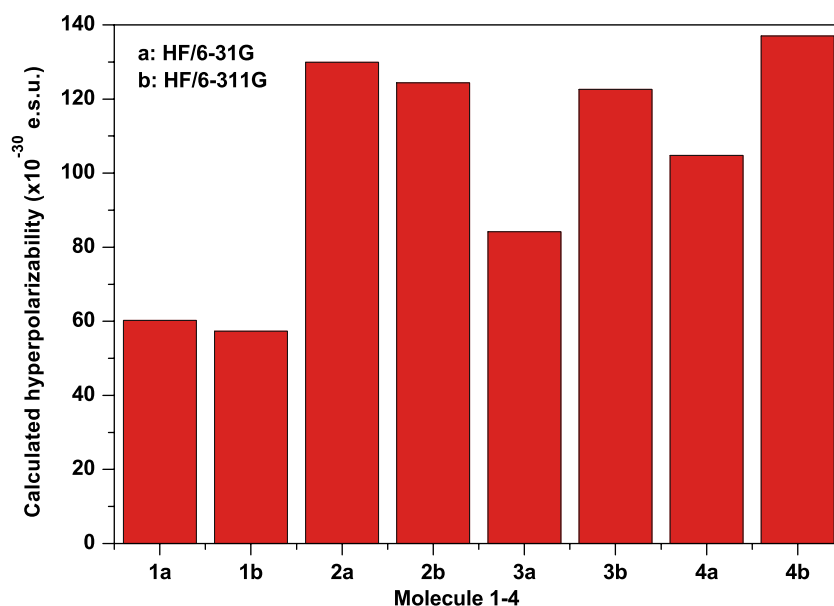
aromatic ground state that enables an aromatic, stabilized and highly polarized charge transfer state. The aromatic tautomers core can be used as an effective π-bridge in the design of new organic NLO molecules. In this study, we report the ground state dipole moment (μ), polarizability (α), anisotropy of polarizability ($\Delta\alpha$), molecular first hyperpolarizability (β) and molecular frontier orbital energy (HOMO, LUMO) of **1–4**. First static hyperpolarizability values (two state model) are indirectly compared to the theoretical results. Calculated results seem to be in a good agreement with experimental ones. The HOMO-LUMO calculations show that the first hyperpolarizability of **1–4** is directly related to the HOMO-LUMO energy gap. The molecule **2** which has the smallest energy gap has the highest first hyperpolarizability while **1** which has the highest energy gap have the smallest first hyperpolarizability.

Fig. 6 Variation of theoretical polarizability and anisotropy of polarizability of molecule **1–4**
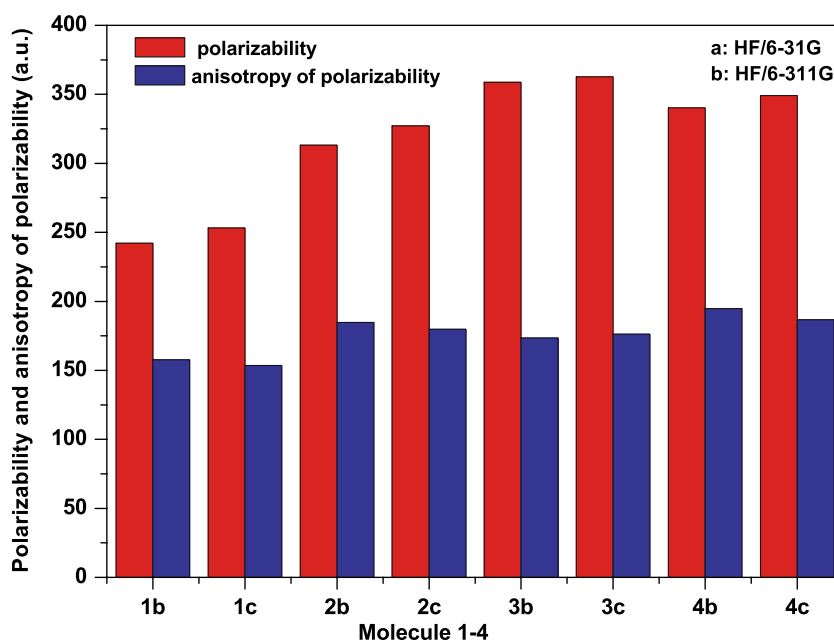
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