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A molecular design view on the first hyperpolarizability of salicylideneaniline derivatives

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Abstract. Electron correlation effect was incorporated into the two-level framework through configuration interaction (CI) calculation including both occupied and unoccupied frontier orbitals, to evaluate the first hyperpolarizabilities of title compounds. Theoretical results are in excellent agreement with experimental data obtained by the solvatochromic method. Some detailed chemical and electronic information of the electron excitation process related to the nonlinear optical (NLO) properties were produced as well. Based on these data, effects of the character, number and position of donor and acceptor groups on the NLO properties are discussed from the viewpoint of molecular design. Not only the experimental data but also the theoretical analysis have suggested that a large number of intensive and properly located donor and acceptor groups may yield the optimal hyperpolarizabilities.

Key words: Salicylideneaniline derivatives – Hyperpolarizability – Solvatochromic method – Two-level model – Charge transfer

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1 Introduction

Nowadays one of the most interesting research topics in the field of material science is that of nonlinear optical (NLO) properties, which has attracted much efforts of both experimental and theoretical scientists [1]. On account of the easy manipulation during the synthesis and the large flexibility for molecular design, organic and organometallic compounds have been the focus for investigation in this realm [2, 3]. Those materials with large second susceptibility $\chi^{(2)}$ associated with the molecular first hyperpolarizability, β, have many potential uses in data storage, telecommunication and information processing. It is found that conjugated organic species with electron donor and acceptor moieties may have a large value of β. Recent studies have revealed [4] that β generally depends on the donor and acceptor strength and the appropriate separation, so long as intense electronic coupling is able to occur through the conjugated bridge. Therefore, the effort to identify optimal hyperpolarizabilities may concentrate on three aspects: search for proper donor, acceptor and conjugated bridge.

Apart from the considerable efforts in experimental work, theoretical scientists have also designed many models to correlate β with some intrinsic molecular properties [5, 6], which is helpful in the molecular design of this kind of substances. In general, the sum-over-state (SOS) and finite-field (FF) approaches are most widely employed in practical calculations [7, 8]. The SOS formula [7] can be expressed as follows:

$$\beta = \frac{1}{2\hbar^2}\left[\sum_{\substack{n,n'\neq g\\ n\neq n'}} \mu_{gn}\mu_{gn'}\mu_{nn'}\frac{3\omega_{gn}\omega_{gn'}+\omega^2}{(\omega_{gn}^2-\omega^2)(\omega_{gn'}^2-\omega^2)} + \sum_{n}\mu_{gn}^2(\mu_n-\mu_g)\frac{3\omega_{gn}^2+\omega^2}{(\omega_{gn}^2-\omega^2)^2}\right] \tag{1}$$

where ω is the angular frequency of the incident laser, μ_g and μ_n are the dipole moments of the ground state (GS) and the excited state (ES) respectively, μ_{gn} and μ'_{gm} are the dipole moments for the transition from GS to different ES, μ'_{nn} is the dipole moment for the transition from one ES to the other, and ω_{gn} and ω'_{gn} are the angular frequencies of the transition from GS to different ES. It should be noted that β essentially is a three-order tensor. The computation value for β without any subscript by Eq. (1) is usually interpreted as the vector component along the dipole moment direction, which sometimes is written as β_μ or β_vec. This notation is used throughout this work.

However, in the alternative widely used FF model [8], the field-dependent dipole moment $\mu(E)$ is expressed as follows;

$$\mu(E) = \mu_i^0 + \sum_j \alpha_{ij}E_j + 1/2\sum_{j,k}\beta_{ijk}E_jE_k + 1/6\sum_{j,k,l}\gamma_{ijkl}E_jE_kE_l + \cdots \tag{2}$$

where E is the external electric field, i, j ,k and l denote coordinates, μ_i^0 is the permanent molecular dipole moment, and α_{ij}, β_{ijk}, and γ_{ijkl} are the tensor elements of the molecular linear, quadratic and cubic polarizabilities, respectively. Then β or β_μ can be obtained by the following equations:

$$\beta = \frac{3}{5}\sum_i \frac{\beta_i \mu_i}{|\mu|} \tag{3}$$

$$\beta_i = \sum_j \beta_{ijj} \tag{4}$$

Both *ab initio* and semi-empirical Hamiltonians, according to the system's magnitude, have been employed to assess the electronic properties which contribute to their hyperpolarizabilities within these two theoretical models. Usually these two methods are in good qualitative and sometimes quantitative agreement with experimental outcome [9, 10].

The SOS method theoretically should have the infinite expansion form which takes account of all excited states by a full-CI technique [11]. However, the rapid convergence of the series expansion for the second-order NLO response justifies the practical significance of truncation. Recently, this method has been explored with various semi-empirical Hamiltonians such as CNDO, INDO and ZINDO on miscellaneous organic and organometallic species [11–13]. Some authors have found that a set of about 50 excited states is sufficiently large in calculation for the first hyperpolarizability.

For simplicity, a two-level model was introduced in the early times of nonlinear optics. As shown in Eq. (5), it is actually a truncation result of the full perturbation theory of Eq. (1) involving only the first excited state:

$$\beta = \frac{3\mu_{eg}^2 \omega_{eg}^2 (\mu_{ee} - \mu_{gg})}{2\hbar^2(\omega_{eg}^2 - \omega^2)(\omega_{eg}^2 - 4\omega^2)} \tag{5}$$

It can give a satisfactory estimation of β where the charge-transfer excited-state term dominates the perturbation summation [4]. This case is usually corresponding to the axially delocalized states. Hence, it is no wonder that the two-level model is able to present a reasonable elucidation for the experimental β values of many organic compounds measured by a dc electric field-induced second harmonic generation (EFISH) method done in solution [14, 15].

The two-level model is generally considered to be too simple to have use in the practical manner as far as quantitative results are concerned [16]. It seems no one has ever incorporated the CI into the two-level model due to its simple formalism. The essence of the two-level model is to use the information of the first possible electron transition between GS and ES to evaluate the NLO properties. This idea may be extended here. As a matter of fact, many molecules can be regarded as the integral of both donor and acceptor parts. In these molecules the donor part is the main component of occupied frontier orbitals (OFO), while the acceptor part is that of unoccupied frontier orbitals (UFO). Therefore, the electron excitation from GS to ES is associated with the electron transfer from the donor part to the acceptor part. In order to include the electron correlation effect, configuration interaction between some OFO and UFO is employed in the operative calculation to produce the new frontier orbitals. After the CI computation, all the new GS and ES have some extents of original OFO and UFO, i.e., each state now has combined appropriate electron correlation from other states. Then, as done by the two-level model, the first possible electron excitation process from the new GS to the new ES is utilized to evaluate β.

Only two levels are used in this simplified approach, in contrast to the higher numbers of levels in the SOS framework. Actually the summation is not performed here. Thus, if it is proved to be effective in the study of NLO properties for certain substances, it must be quite attractive by reason of its fairly inexpensive and efficient computation. Its attractiveness also lies in the fact that it can provide some helpful electronic information for molecular design. This was tested by estimating the β values of several salicylideneaniline derivatives in this paper, where the experimental first hyperpolarizabilities were obtained by our previous solvatochromic measurement. In order to obtain some useful guidelines for molecular design, the effect of the nature, number and position of donor and acceptor groups on the first hyperpolarizability was discussed because the conjugated bridege of the studied compounds here is the same.

2 Computational approach

In general, the component β_x (x is the direction of the applied dc electric field) can be easily used to evaluate the second harmonic generation (SHG) effect. This value can be measured by EFISH method [15]. In fact, if the external electric field is applied in the direction of the molecular dipole moment, β_x has the same value as β_μ. On the other hand, another important experimental technique, called the solvatochromic method [17] can be employed to obtain β_{xxx}. The relation between these two terms is expressed as follows:

$$\beta_x = \beta_{xxx} + 1/3(\beta_{xyy} + \beta_{yxy} + \beta_{xzz} + \beta_{zxz}) \tag{6}$$

It is shown by experimental data [17] that β_{xxx} is the outweighing component in the evaluation for β_x by the above equation and that the tendencies in these two quantities are very consistent. Therefore, β_{xxx} can be used as well as β_x in the assessment of the relative merit of some organic compounds. In addition, β is a function with respect to the off-resonant frequency (ω) of the incident laser beam as described below [18]:

$$\beta_{\omega=0} = \beta_\omega[(\omega_{eg}^2 - 4\omega^2)(\omega_{eg}^2 - \omega^2)/\omega_{eg}^4] \tag{7}$$

In this work, all β values refer to the zero-frequency level if not explicitly stated.

As depicated in the Introduction, the present method does not make use of the original highest occupied molecular orbital and lowest unoccupied molecular orbital directly. No matter how many states are generated from the CI calculation (certainly with more OFO and UFO, more states can be obtained), the present approach takes advantage of just two states, one GS and one ES, in the new orbital space. For instance, three OFO and three UFO are involved in the current CI computation, from which 19 configurations are obtained. But all the quantities which are necessary to the evaluation of the first hyperpolarizability are relevant to these two states which produce the first possible electron transition. Then β can be obtained on the basis of Eq. (5) as follows:

$$\beta = C\lambda_{eg}^2\mu_{eg}^2(\mu_{ee} - \mu_{gg}) \tag{8}$$

where λ_{eg} is the excitation wavelength, and C is a constant with the value 3.79597×10^{-7} when the units of th first hyperpolarizability, excitation wavelength, and dipole moments are in 10^{-30} esu, nm and debye respectively.

As shown in Fig. 1, four salicylideneaniline derivatives of the donor-acceptor type are studied here. These compounds were selected because of their distinct thermochromatic or photochromatic behaviours, which has already induced much interest on the part of materials scientists [19, 20]. Because the crystal structure is available only for molecule **B** [21], for consistency, all these geometries were generated by the model-builder of the software HyperChem [22]. Then they were optimized on a SUN workstation by MOPAC (version 6.0). The singly-excited CI calculation was performed by HyperChem on the optimized molecular structures. In all quantum chemical calculations, the semi-empirical AM1 [23, 24] Hamiltonian was employed. The self-consistent-field convergence criterion was set as 10^{-8} a.u. together with the keyword "PRECISE" in all MOPAC computations. When the gradient is less than 0.01 Kcal/(mol Å), the optimization process will stop. There is no symmetry constraint during the optimization process The semi-empirical parameters for H, C, N, O, Cl and Br in all calculations are set by the program default [23, 25].

3 Experimental and theoretical results and discussion

The experimental values of β_{xxx} for the studied compounds determined by solvatochromic technique in different solvents [26] was reported previously. All the values were measured with the incident laser beam at frequencies 1064 and 1907 nm as usual. They are listed in Table 1 as β(1064 nm) and β(1907 nm) respectively. In order to compare them with the theoretical results, they were transformed into zero-frequency level according to Eq. (7), as denoted by β_0(1064 nm) and β_0(1907 nm) respectively. It can be seen that these two data are very close for a specific compound. β_0 is the mean value of these two data in each solvent. As shown in Table 1, each compound does not have a unique β_0 in different solvents. Nevertheless, among all values of β_0 for one compound in seven solvents, there is merely one deviating largely from others. Thus the average of the other six similar data is used as the representative value for the specific compound, which is written as β_{exp} in Table 1 to be compared with the computational consequence later.

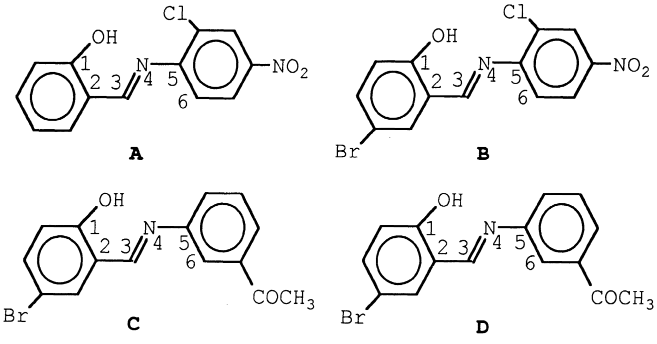

Fig. 1. Molecular structures of the studied compounds

This system is typified by the presence of hydrogen bond O—H···N, which is also responsible for their special chromatic properties [19]. The study on the correlation between the proton-transfer from the oxygen part to the nitrogen part and the configuration change from the enol-form to the keto-form is of great theoretical interest [27]. It may be significant in governing the compound's physical and chemical properties. Obviously, the planarity and conjugative properties of these molecules containing the —C=N— may be destroyed partially by the formation of the hydrogen bond, which makes all of their β values not very large compared with those compounds containing the —C=C— bond.

The partial breakdown of the planarity of title compounds can be exemplified by the twist angles listed in Table 2. The twist angle denotes the twist information of the nitroaniline ring relative to the other phenyl ring, which is the sum of two dihedral angles ∠1–2–3–4 and ∠3–4–5–6. Here, ∠1–2–3–4 can describe the twist of the salicylidene ring relative to the azomethine group, while ∠3–4–5–6 is the dihedral angle of the aniline ring plane and the azomethine group plane. As seen from Table 2, the substitution affects the twist of the aniline part more significantly than that of the salicylidene part. The twist angles of compounds **A** and **B** are much larger than those of compounds **C** and **D**. This may be due to the steric effect of the chlorine substituent like in the case of *N*-tetrachlorosalicylideneaniline [28]. Because this group is very near the hydrogen-bonded nitrogen atom, it may easily influence the hydrogen bond as well as the planarity of the molecule. The twist angle of compound **C** is also much larger than that of compound **D**. Such phenomena may be explained by the presence of the more favorable conjugation site of —$COCH_3$. The effect of the conformation on the first hyperpolarizability is well known. Our previous work [29] on some donor-acceptor type molecules shows that they usually have low-barrier rotation modes and β is sensitive to conformation. The largest β happens with the planar conformation. As regards the compounds studied here, the rotation barriers between the planar and the optimized conformation are also very small: 1.2, 1.4, 1.1 and 0.1 kcal/mol for molecules **A**, **B**, **C** and **D** respectively. This order is the same as that of the twist angles. The first hyperpolarizabilities at the planar conformation are 12.48, 18.26, 4.63 and 7.26×10^{-30} esu for **A**, **B**, **C** and **D** respectively. Compared with those values at the optimized geometries (see

Table 1. Experimental data for the first hyperpolarizability

No.	Solvent	β(1064 nm)	β_0(1064 nm)	β(1907 nm)	β_0(1907 nm)	β_0	β_{exp}
A	1	55.47	26.63	32.20	26.63	26.63	10.56
	2	20.72	9.13	11.23	9.13	9.13	
	3	22.84	10.78	13.08	10.78	10.78	
	4	22.15	10.26	12.53	10.28	10.27	
	5	23.49	10.85	13.10	10.75	10.80	
	6	21.53	10.05	12.23	10.05	10.05	
	7	25.15	12.33	14.85	12.33	12.33	
B	1	18.87	8.46	10.34	8.43	8.45	14.39
	2	30.44	13.33	16.42	13.33	13.33	
	3	27.27	13.02	15.76	13.02	13.02	
	4	29.73	14.04	17.08	14.08	14.06	
	5	28.84	13.84	16.74	13.84	13.84	
	6	32.11	15.25	18.48	15.25	15.25	
	7	34.13	16.82	20.23	16.82	16.82	
C	1	11.80	5.88	7.05	5.88	5.88	5.50
	2	11.06	5.37	5.89	4.88	5.12	
	3	12.79	6.37	7.65	6.37	6.37	
	4	4.39	2.22	2.65	2.22	2.22	
	5	10.25	5.13	6.15	5.13	5.13	
	6	9.25	4.73	5.64	4.73	4.73	
	7	11.28	5.76	6.88	5.76	5.76	
D	1	–	–	–	–	–	8.01
	2	17.18	8.20	9.93	8.20	8.20	
	3	17.06	8.28	9.99	8.28	8.28	
	4	13.73	6.77	8.14	6.77	6.77	
	5	16.89	8.33	10.01	8.32	8.33	
	6	17.03	8.48	10.18	8.48	8.48	
	7	4.03	1.93	2.34	1.93	1.93	

All β values are in the unit of 10^{-30} esu. Solvents are denoted as follows:
1, cyclohexane; 2, toluene; 3, ether; 4, ethyl acetate; 5, acetonitrile; 6, cyclohexanone; 7, ethanol

Table 2. Twist angles of title compounds

Compound	A	B	C	D
∠1–2–3–4 (°)	−4.39	−4.23	−4.87	−1.11
∠3–4–5–6 (°)	36.21	39.02	21.99	4.11
Twist angle (°)	31.82	34.79	17.12	3.00

Table 3. Charge distribution of both ground (g) and excited (e) states

Group		A	B	C	D
q_N	g	−0.219	−0.210	−0.200	−0.214
	e	−0.144	−0.150	−0.193	−0.177
q_o	g	−0.250	−0.244	−0.249	−0.251
	e	−0.225	−0.220	−0.223	−0.229
q_{cl}	g	0.028	0.029	–	–
	e	0.046	0.049	–	–
q_{Br}	g	–	0.064	0.057	0.058
	e	–	0.082	0.068	0.068
q_{NO_2}	g	−0.139	−0.135	–	–
	e	−0.175	−0.170	–	–
q_{COCH_3}	g	–	–	0.021	0.022
	e	–	–	0.025	−0.001

Table 4), great enhancement of β takes place in the case of a large difference between two conformations. As a result, the enhancement of β also follows the order **B** > **A** > **C** > **D**. However, the relative strength of the second NLO response for these compounds does not change.

In order to understand the nature of charge transfer, electron population analysis of both ground and excited states was performed. The charge distribution for all the substituents and the hydrogen-bonded oxygen and nitrogen atoms are shown in Table 3. Based on the amount of the charge variation, it can be found that the hydrogen-bonded oxygen and nitrogen atoms are strong donors, while the halogen substituents —Cl and —Br are weak donors. As regards the acceptors, the group —NO_2 is more intensive than the group —$COCH_3$ because the former can withdraw several times more electrons than the latter.

As far as these four molecules are concerned, a ranking of the chemical effect on the order of **B** > **A** > **D** > **C** for the first hyperpolarizability can be established. As shown in Fig. 1, current compounds have the identical conjugation backbone. Therefore, only the effects of proper donor and acceptor groups on the hyperpolarizability are discussed. Three effects, i.e., the character, number, and position of the donor and acceptor parts, should be taken into account in order to optimize β. It has been found [4] that large β happens in the molecule with significant charge-transfer between donor and acceptor groups. This phenomenon usually is connected with strong donor and acceptor substituents. It is well known that the —NO_2 group is a more intensive acceptor than the —$COCH_3$ group, as illustrated in Table 3. In fact, it is the major reason for the fact that the β data of compounds **A** and **B** are larger than those of compounds **C** and **D**. This indicates the significant effect of the nature of the donor or acceptor group. The fact that β_{exp} of compound **B** is greater than that of compound **A** may be due to the existence of another donor, —Br, in compound **B**. This case shows that when more donor or acceptor groups are involved in the substance, its NLO response may be enhanced. The location of the donor and acceptor groups affects the NLO properties through the influence on the conjugation. As described in Eq. (8), the wavelength λ_{eg} is also an important factor in governing the first hyperpolarizability. If the donor part and acceptor part are more chemically conjugated, λ_{eg} and the consequential β will be larger. By virtue of comparing the para- and ortho- positions of —$COCH_3$ acceptor in phenyl ring with respect to the donor portion, the larger β value of **D** than that of **C** may be explained. Therefore, besides the nature and number of donor and acceptor groups, the position of a given substituent is also of vital importance for molecular design in this field. Although the larger twist angles of compounds **A** and **B** than of compounds **C** and **D** may reduce the conjugation effect, the first hyperpolarizabilities of the former are still larger than those of the latter. This indicates that the effect of the nature and number of donor and acceptor groups may be greater than that of the conjugation.

Theoretical methods can provide another pathway into this appealing research field [6]. As shown in Table 4 and Fig. 2, the predicted values, β_{cal}, based on AM1/CI calculations are close to the experimental data. The current approach can reproduce the correct order of the four experimental β values. The good linear relationship between the computational and experimental results is exemplified by the excellent correlation coefficient of 0.98. Therefore, the present method, though it is simple in formalism, can provide accurate results in the investigation of certain donor-acceptor type compounds.

Table 4. Computational results of β_{cal}

Compound	μ_{gg}	μ_{ee}	μ_{eg}	λ_{eg}	β_{cal}
A	6.65	10.49	7.59	341.6	9.80
B	4.94	9.84	8.05	333.6	13.41
C	1.68	2.65	7.78	320.2	2.29
D	3.31	5.65	8.70	327.9	7.23

The units for μ, λ and β here are debye, nm, and 10^{-30} esu respectively

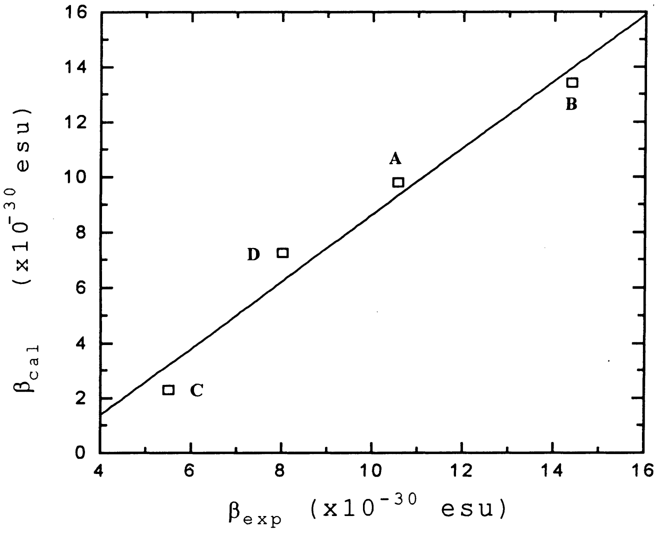

Fig. 2. The relationship of β_{cal} and β_{exp}

It can be seen from Table 4 that when the donor or acceptor groups change, they will affect the ground and excited-state dipole moments more than other physical quantities. The effect of different acceptor groups can yield the larger excitation wavelengths in compounds **A** and **B** compared to compounds **C** and **D**. The presence of —Cl and —NO_2 groups in compounds **A** and **B** has produced the larger polarization due to their relatively strong electron-withdrawing nature, and given rise to the larger dipole moments of both ground state and excited state than those of compounds **C** and **D**. The two effects contribute together to the larger hyperpolarizabilities. In compound **C**, —$COCH_3$ group is in the unfavorably conjugated location, which is responsible for the smallest value of λ_{eg}. Such unfavorable conjugation may result in an elevated energy gap between the occupied and unoccupied level.

4 Conclusion

It is well known that the electron correlation effect is quite significant in theoretical consideration for the evaluation of the nonlinear optical properties. The inclusion of electron correlation has been highly recommended by several authors [30–32]. There is sometimes quite a large difference between the hyperpolarizabilities calculated with and without electron correlation for large molecules such as *p*-nitroaniline by *ab initio* study [31]. Therefore, it is no wonder that the consideration of this effect enables the present simple method to produce excellent quantitative results. In addition, this procedure can provide more detailed electronic information on the studied substances, which helps us to gain deeper insight into their chemical and physical properties. Both experimental and theoretical information show that the substituent effect (including the nature, number and position) is of considerable importance in the determination of the NLO properties. On the basis of the current study, it may be concluded that a large number of intensive and properly located donor and acceptor groups may yield the optimal hyperpolarizabilities from the viewpoint of molecular design engineering.

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