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TWO-PHOTON ABSORPTION ACTIVITIES OF SYMMETRIC/ASYMMETRIC LINEAR MOLECULAR SYSTEMS CONTAINING AZO AND DIACETYLENE MOIETIES AS CENTRAL π-BRIDGE

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Two-photon absorption (TPA) properties of several linear molecules were experimentally studied and discussed in terms of their π-bridge. Asymmetric molecules containing C=C, N=N, and N=C π-bridges were examined and found that molecular planarity along the π-bridge plays an important role on TPA activity. Also symmetric bis(styrylpyridines) derivatives containing a diacetylene π-bridge were examined and found to exhibits stronger TPA than the aromatic π-bridge molecule with similar extent of π-conjugation. Drastic enhancement of TPA cross section due to resonance enhancement was also found for one of the diacetylene compounds in visible wavelength region.

Keywords: azobenzene; diacetylene; π-bridge; stilbene; resonance enhancement; two-photon absorption

INTRODUCTION

Two-photon absorption (TPA) property of organic materials has attracted considerable interest in the last several years because of its growing applications in the fields of photonics [1–5], biophotonics [6–8], and medicine [9]. For these applications, a common requirement to the materials is high TPA activity. Thus, a lot of efforts have been devoted to develop TPA chromopheres with large TPA cross section $\sigma^{(2)}$ that matches practical requirements of the applications. Among a number of strategies of

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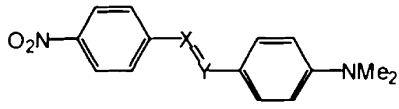
molecule design proposed for this aim, the basic structure is a combination of electron rich (donor, D) or deficient (acceptor, A) terminal substituent groups linked with π-conjugation bridges (π) in symmetric (D$-\pi-$D, A$-\pi-$A) or asymmetric (D$-\pi-$A) ways. The influence of the D and A strength of terminal groups and symmetry of their arrangement on TPA activity have been extensively studied [10–14]. Contrary to this, limited attention has seemed to be paid to nature of π-bridge [12,15].

The aim of this paper is throwing light on the relationship between structure of π-bridge and TPA activity. Most structures of π-bridge reported to date are based on linear and aromatic C=C double bonds, such as vinylene, phenylene (or phenylenevinelne) [10,11], fluorene [12,13], dithienothiophene [14,15], etc. These π-bridges consist of carbon atoms having sp^2 hybrid orbitals. On the other hand, other forms of π-bridges can be possible. One example is double bonds containing sp^2 nitrogen atoms: i.e. N=N and N=C, and another is a triple bond containing sp carbon atoms. In this paper, we discuss TPA properties of molecules containing these two kinds of π-conjugation structures as π-bridge. As the first series, four molecules were investigated, which have the same terminal substituent groups but differ in their π-bridge (Fig. 1, Series I): A (p-nitrophenyl) and D (p-dimethylaminophenyl) groups are linked in an asymmetric way by X = Y π-bridges (X, Y = C, N). Here the molecules are labeled as **AC** = **CD** (4-dimethylamino-4′-nitrostilbene), **AN** = **ND** (4-dimethylamino-4'-nitroazobenzene), **AC** = **ND** (4-dimethylamino-*N*-(4-nitrobenzylidene)aniline), and **AN** = **CD** (4-nitro-*N*-(4-dimethylaminobenzylidene)aniline). Another series consists of molecules containing a diacetylene moiety as a π-bridge (Fig. 1, Series II). They have 4-styrylpyridine derivatives as terminal substituents arranged in a symmetric way. An interesting point of triple bonds is that they brings moderate π-electronic communication through the π-bridge without large red-shift of linear absorption bands [16]. The three molecules containing a diacetylene π-bridge (**MPPBT**, **PPBT**, and **MPPB**) are different each other in their pyridine/pyridinium forms and in methoxy side chains. A molecule with the same substituent groups but containing an aromatic C=C π-bridge (**MPBT**) was also studied for comparison. TPA absorption spectra of these series of molecules were measured by the femtosecond open aperture Z-scan method. For each series, direct comparison was made among molecules on the relation between structure of the π-bridges and their TPA activities.

EXPERIMENTAL

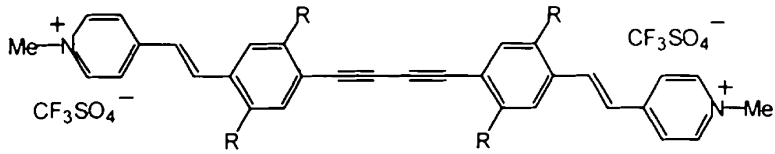
The preparation of the compounds used for the experiments were reported elsewhere [17,18]. All compounds were dissolved in spectroscopic grade DMSO and used as samples. The concentrations were 1–5 mM for all

Series I

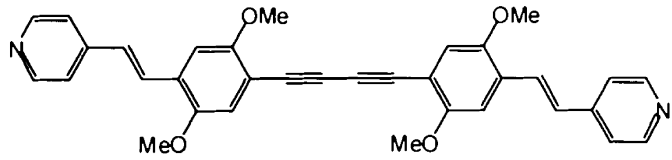


Compound	X	Y
AC=CD	C	C
AN=ND	N	N
AC=ND	C	N
AN=CD	N	C

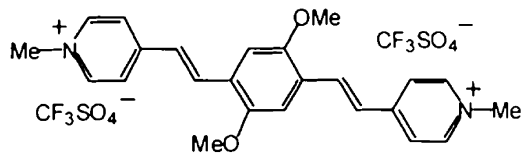
Series II



R=OMe (**MPPBT**), H (**PPBT**)



MPPB



MPBT

FIGURE 1 Molecular structures of compounds studied.

compounds. TPA spectra were measured by open aperture Z-scan method. The details of our experimental setup reported previously [17,19,20]. A femtosecond optical parametric amplifier (*Spectra-Physics OPA-800*) pumped by a regenerative amplifier system (*Spectra-Physics Spitfire,*

Merlin, Tsunami, Millennia) operating at 1 kHz was used as light source. At each wavelength, open aperture traces were recorded for several different incident powers and were analyzed with the reported method where the incident pulses are assumed to be spatially and temporally Gaussian [21,22]. Proportional relation between TPA parameter q_0 and on-axis peak intensity at the focal point I_0 was confirmed for every measurement, exhibiting that the effect of higher-order nonlinear absorption processes such as excited state absorption (ESA) and three-photon absorption (3PA) were negligible for the power range applied (0.1–0.6 mW), corresponding to an I_0 range of $30 \sim 300$ GW/cm^2 depending on the experimental conditions such as wavelength, beam divergence, and pulse width. TPA cross section $\sigma^{(2)}$ was obtained from the convention of $\sigma^{(2)} = (hc/\lambda)(\alpha^{(2)}/N)$, where N is number density, hc/λ is photon energy at the incident wavelength λ, and $\alpha^{(2)}$ is TPA coefficient, which obtained from analysis of the open aperture traces.

RESULTS AND DISCUSSION

π-Bridge Containing sp^2 Nitrogen Atoms

TPA spectra of the four molecules in Series I are shown in Figure 2. TPA bands were found for all compounds around 880–970 nm. The peak values of $\sigma^{(2)}$ were similar for **AC** = **CD** (191 ± 10 GM*) and **AN** = **ND** (178 ± 23 GM), but smaller for *N*-benzylideneanilines (**AC** = **ND**: 133 ± 7 GM; **AN** = **CD**: 76 ± 7 GM). Among these four molecules, the terminal substituents and their arrangement are the same, so the difference originates only from structural difference of the π-bridge. There is no significant difference in the $\sigma^{(2)}$ value for **AC** = **CD** and **AN** = **ND**, suggesting that sp^2 carbon and sp^2 nitrogen atoms themselves have similar ability as π-bridge. Therefore, the smaller values of the *N*-benzylideneanilines must be related with other factors rather than difference in element. A reasonable explanation is planarity of the molecules. Although the X-ray data for **AC** = **CD** and **AN** = **ND** have not been reported, there is little doubt that they are expected to be planer from the X-ray data for the related structures and the theoretical calculations [24–27]. Meanwhile, *N*-benzylideneanilines are considered as nonplaner. It is reported that **AN** = **CD** is twisted by 45° around C(phenyl)-N bond in solid state [28,29]. Therefore, the weak TPA of **AN** = **CD** can be related to the nonplaner structure, which reduces delocalization of electron through the π-bridge. The planarity of other isomer, **AC** = **ND**, remains a question because the crystallographic data [28] and the quantum chemical calculations still contradict each other [25,30,31].

*1 GM = 10^{-50} cm^4 s molecule^{-1} photon^{-1}.

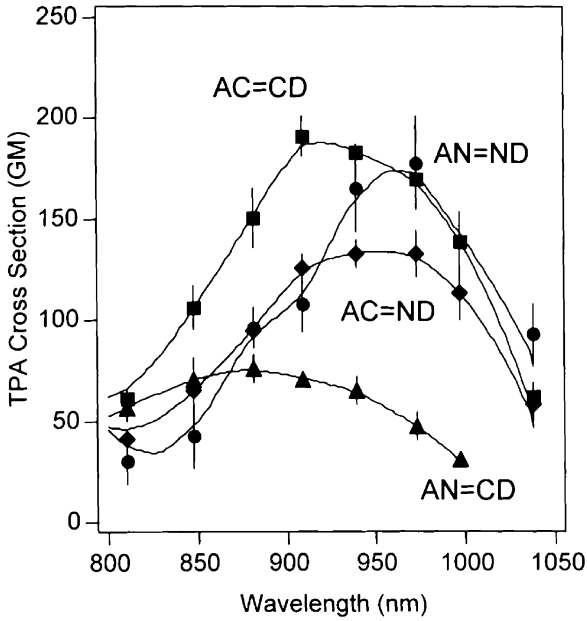


FIGURE 2 Two-photon absorption spectra of the compounds in Series I (**AC** = **CD**: square, **AN** = **ND**: circle, **AC** = **ND**: diamond, **AN** = **CD**: triangle).

The TPA intensity of **AC** = **ND** are moderate in the four compounds, so it probably deviates somewhat from a planer structure.

The peak wavelengths of the TPA bands were found to be almost twice the peak wavelengths of their linear absorption bands (Table 1). The TPA transitions are considered to occur to the same final states as their one-photon absorption because parity selection rule does not hold for

TABLE 1 One- and Two-Photon Absorption Properties of the Compounds in Series I

	One-photon		Two-photon			
Compound	$\lambda^{(1)}$/nm	ε/M^{-1}cm^{-1}	$\lambda^{(2)}$/nm	$\sigma^{(2)}$/GM	$M_{ge}{}^{a}$/D	$\Delta\mu_{ge}{}^{b}$/D
AC = **CD**	452	26 900	909	191 ± 10	7.4	19
AN = **ND**	501	33 100	973	178 ± 23	7.6	17
AC = **ND**	460	17 500	939	133 ± 7	6.1	16
AN = **CD**	416	27 000	881	76 ± 7	6.7	15

[a] Calculated from oscillator strength obtained from one-photon absorption spectrum by assuming Gaussian band profile, [b] determined by absorption electrochromism [32].

asymmetric molecules. Therefore, the TPA transitions of these molecules can be explained by taking account of at least two states: the ground state and the lowest excited state that is both one- and two-photon-allowed state. In this two-state model, the peak value of TPA cross section $\sigma^{(2)}_{peak}$ can be related to the transition energy E_{ge}, the transition dipole moment M_{ge}, and difference in dipole moment between the ground and the excited states $\Delta\mu_{ge}$ with the following theoretical Equation (17):

$$\sigma^{(2)}_{peak} \propto \frac{M^2_{\mathrm{ge}}\Delta\mu^2_{\mathrm{ge}}}{E^2_{\mathrm{ge}}} \tag{1}$$

A plot of the observed $\sigma^{(2)}_{peak}$ against the right-hand-side quantity of Eq. (1) calculated from experimental and reported values (Table 1) is presented in Figure 3. All molecules except **AC** = **ND** falls on a proprtional line, suggesting the two-state model (Eq. (1)) works well for the three molecules. As in the discussion of planarity, **AC** = **ND** alone deviates from the straight line. This is due probably to that any other factors not considered in Eq. (1) contribute to the peak $\sigma^{(2)}$ value of **AC** = **ND**. However, it is worth to be noted here that TPA properties of these asymmetric molecules can be basically predicted from their one-photon absorption properties because one- and two-photon transitions occurs to the same excited state.

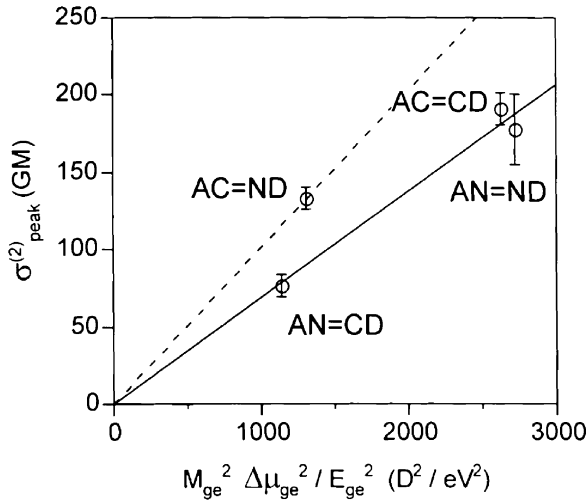


FIGURE 3 Correlation between the experimentally obtained peak values of TPA cross section and calculated value of $M_{\mathrm{ge}}{}^2\,\Delta\mu_{\mathrm{ge}}{}^2/E_{\mathrm{ge}}{}^2$, for the compounds in Series I. See text for details.

π-Bridge Containing *sp* Carbon Atoms

TPA spectra of the molecules containing a diacetylene π-bridge (**MPPBT**, **PPBT**, **MPPB**) are shown in Figure 4. Intense TPA bands were observed around 690–760 nm for all molecules. Comparison among the three molecules containing diacetylene π-bridge shows that both quarternization of the pyridyl groups and methoxy substitution of phenylene groups enhance TPA activity as well as improve solubility. The largest value of the peak $\sigma^{(2)}$'s at the TPA bands was found for **MPPBT** (848 ± 96 GM at 764 nm).

On the other hand, the peak value for **MPBT** was less than a half of that of **MPPBT**. **MPBT** has the same terminal substituents as **MPPBT** but has a phenylene type π-bridge instead of a diacetylene π-bridge of **MPPBT**. The peak wavelength of one-photon absorption is almost the same as that of **MPPBT** (Table 2), suggesting extent of π-conjugation is similar for both molecules. The fact that **MPPBT** exhibits more intense TPA than **MPBT**, in spite of the similar extent of conjugation for them, suggests the usefulness of diacetylene π-bridge for larger TPA activity. It is speculated that a weak coupling of π-electronic communication through triple bonds may enhance TPA cross section, as in the case of branched molecules [33].

The peak wavelengths of the TPA bands were found to be red-shifted by $90 \sim 100$ nm from twice those of one-photon bands for all molecules. The difference is too large to be explained with change of vibronic coupling between one- and two-photon transitions. Unlike the molecules in Series I, the molecules in Series II have symmetric structure along the molecular

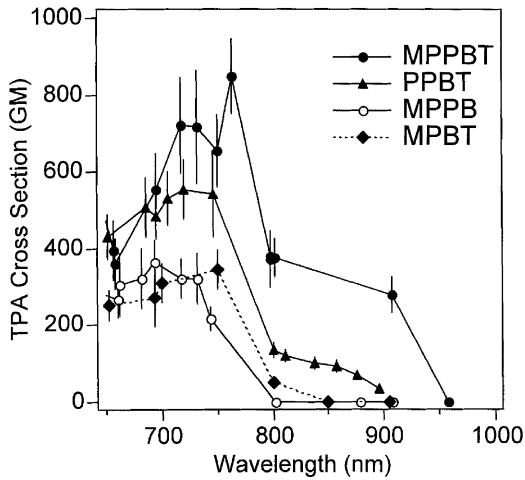


FIGURE 4 Two-photon absorption spectra of the compounds in Series II.

TABLE 2 One- and Two-Photon Absorption Properties of the Compounds in Series II

	One-photon		Two-photon	
Compound	$\lambda^{(1)}$/nm	ε/M^{-1}cm^{-1}	$\lambda^{(2)}$/nm	$\sigma^{(2)}$/GM
MPPBT	467	66 700	764	848 ± 96
			(571)	$(2\ 420 \pm 460)^a$
PPBT	397	88 400	720	554 ± 79
MPPB	421	71 400	694	363 ± 56
MPBT	462	36 200	751	346 ± 51

[a] Not at a peak. See text for details.

axes; therefore, the parity selection rule holds and the TPA transition occurs to a one-photon-forbidden excited state.

Moreover, as the incident wavelength decreased below 650 nm, the $\sigma^{(2)}$ values exhibited monotonic increase. The increase was drastically for **MPPBT;** its $\sigma^{(2)}$ value reached to 2420 ± 460 GM at 571 nm, which is a huge value as molecules of this size. This drastic increase can be considered to originate from resonance enhancement of TPA due to a one-photon transition because it was found at wavelength near its one-photon absorption band. So, we tried to explain the drastic increase by taking account of four states: the ground state (0), the lowest one-photon-allowed excited state (j), the lowest and second lowest TPA-allowed excited states (f_1 and f_2, respectively) The following formula for TPA cross section was led based on the Sum-Over-State expression with the four states: [23]

$$\sigma^{(2)}(\nu_p) \propto \frac{\nu_p^2}{(\nu_{j0} - \nu_p)^2 + \Gamma_{j0}^2} \left[\frac{A_1}{(\nu_{f_1 0} - 2\nu_p)^2 + \Gamma_{f_1 0}^2} + \frac{A_2}{(\nu_{f_2 0} - 2\nu_p)^2 + \Gamma_{f_2 0}^2} \right], \quad (2)$$

where ν_p is the frequency of incident laser light; ν_{j0}, $\nu_{f_1 0}$, and $\nu_{f_2 0}$, are transition frequencies from 0 to j, f_1 and f_2, respectively; Γ_{j0}, $\Gamma_{f_1 0}$, and $\Gamma_{f_2 0}$ are relaxation constants of the transitions between them; A_1 and A_2 are amplitude factors defined as $A_1 = |\mu_{f_1 j}|^2 |\mu_{j0}|^2 \Gamma_{f_1 0}$ and $A_2 = |\mu_{f_2 j}|^2 |\mu_{j0}|^2 \Gamma_{f_2 0}$ with transition moments μ_{mn} between the states ($m = f_1, f_2$, $n = j$, 0). With the experimental values for ν_{j0}, $\nu_{f_1 0}$ and Γ_{j0}, and assuming $\Gamma_{j0} = \Gamma_{f_1 0} = \Gamma_{f_2 0}$, the four-stare model based on Eq. (2) can successfully reproduce the observed drastic increase as well as the TPA bands at the longer wavelength region (Fig. 5). On the other hand, a three-state model in which the second term in Eq. (2) is omitted cannot be reproduced the features of the observed TPA spectrum. These results show that, at wavelengths below 650 nm, the photon energy of incident laser light increases and

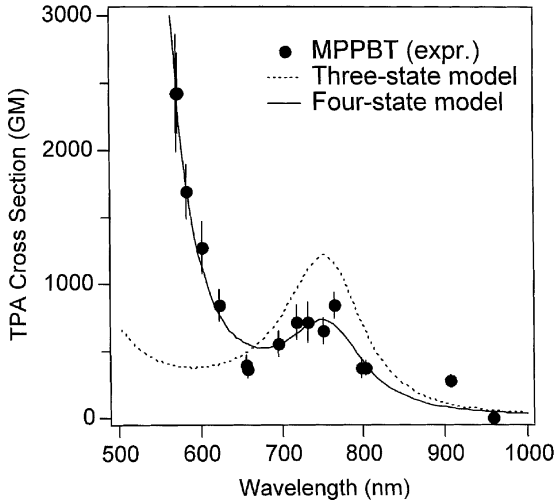


FIGURE 5 Enhancement of TPA cross section of **MPPBT** in visible wavelength region.

TPA transition occurs to the second lowest TPA-allowed states f_2. At the same time, the virtual state of the TPA transition approaches to the lowest one-photon-allowed excited state j, so the transition probability of $f_2 \leftarrow 0$ transition is greatly enhanced. Due to this double resonance, *i.e.* a resonant transition to the second lowest TPA-allowed excited state which is enhanced by near one-photon resonance, the TPA cross section is drastically enhanced in the short wavelength region. It is worth noting here that the virtual state is close to the lowest one-photon excited state but dose not overlap with it. Therefore, contrast of TPA against one-photon absorption is still kept to be very high, which is an important factor for practical applications.

CONCLUSION

In this paper, the role of π-bridge on TPA activity of linear π-conjugate molecules was investigated. For X=Y π-bridges (X, Y are C, N; Series I), extent of π-conjugation controlled by molecular planarity is found to play an important role rather than difference in element in the π-bridges (C or N). The less intense TPA of the compounds with N=C π-bridge can be explained with their poor planarity. Single substitution of a C atom with a N atom in C=C π-bridge cause a bias in electron distribution, which increase single bond character in a bond and allows the molecule to lose

its planarity. The molecules in Series I were linear molecules with a strong donor and acceptor arranged in asymmetric way (A−π−D), so TPA occurs to the same excited state as for the one-photon transition. TPA properties of such asymmetric molecules can be predicted, in some extent, from their one-photon absorption properties.

Contrary to the replacement of C=C with N=N, the replacement with a diacetylene π-bridge made considerable difference in their TPA properties. The compounds with a diacetylene π-bridge in Series II exhibited intense TPA bands in near IR region (690–760 nm). **MPPBT** showed much more intense TPA band than the aromatic π-bridge molecule with the same extent of π-conjugation (**MPBT**), suggesting effectiveness of diacetylene π-bridge for larger TPA activity. Moreover, drastic increase in TPA cross section was found for **MPPBT** in visible wavelength region. This drastic increase was explained with double resonance: enhancement of a TPA transition by near resonance of a one-photon transition. A use of this assistance of one-photon resonance enhancement can be a new strategy of molecular design for materials having huge TPA cross section.

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