Correlations of the 0–0 Transitions, the Absorption and Fluorescence Maxima with the σ-Hammett Constants

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The correlations of the 0–0 transitions, the absorption and the fluorescence maxima with the σ-Hammett constants are established for series of substituted compounds of various structures. The experimental results are analyzed in terms of the changes of the energy gaps between ground and excited states and their force constants upon substitution. On this basis, both the equally and oppositely directed shifts of the maxima of absorption and fluorescence, respectively, are understood.

1. Introduction

In a previous paper [1] an approach for the analysis of correlations between electron transition energies and σ-Hammett constants [2] was developed. The basic assumption in this approach is that the changes in the electron energy obey the principle of "linear free energy relationships" (LFER) [3, 4, 5]. In [1] the fluorescence maxima were correlated for the first time with the σ_X-Hammett substituent constants.

The linear correlations between the absorption frequencies ν^{A}, the fluorescence maxima, ν^{F}, the corresponding 0–0 transitions, ν^{00}, and the σ-Hammett constants, σ_X, allow, in the range of the approach developed in [1], for some important results. The most significant of them is the possibility of separating the effect of the substituent on the Frank Condon (FC) transitions into two independent contributions:

(i) change of the energy gap between the ground (S_0) and excited (S_1) state;

(ii) change of the steepness of the hypersurfaces of S_0 and S_1.

Moreover, from the σ_X correlations the fluorescence maxima positions could be predicted for some representatives of a class which cannot be easily synthesized. The purpose of the present paper is to analyse the interpretative power of the model proposed in [1] by means of $\nu_X - \sigma_X$ correlations obtained experimentically.

The σ-Hammett constants correlate with the electron spectra frequencies less often [6, 7] than with other quantities in physical organic chemistry, e.g. rate and equilibrium constants [4]. For that reason in [1] and in this paper first of all we had to prove that ν^{A}, ν^{F} and ν^{00} correlate linearly with σ_x in different classes of organic compounds.

To avoid repetitions of quoting equations from [1] in the following discussion, we shall give again the basic relations:

$$\begin{aligned} &\Delta\nu = \nu(X) - \nu(\mathrm{H}); \\ &\Delta\nu^{00} = \varrho_{00}\,\sigma_X; \quad \Delta\nu^{\mathrm{A}} = \varrho_{\mathrm{A}}\,\sigma_X; \\ &\Delta\nu^{\mathrm{F}} = \varrho_{\mathrm{F}}\,\sigma_X, \end{aligned} \tag{1}$$

where

$$\varrho_{00} = \frac{1}{h}\left[\left(\frac{\partial E_1{}^0}{\partial_X}\right)_{\mathrm{H}} - \left(\frac{\partial E_0{}^0}{\partial_X}\right)_{\mathrm{H}}\right]; \tag{2}$$

$$\varrho_{\mathrm{A}} = \varrho_{00} + \varkappa_1; \quad \varrho_{\mathrm{F}} = \varrho_{00} - \varkappa_0 .$$

$E_0{}^0$ and $E_1{}^0$ are the zero vibrational level energies of S_0 and S_1,

$$\begin{aligned} \varkappa_1 &= \varrho_{\mathrm{A}} - \varrho_{00} \cong \frac{1}{2h}(R_1 - R_0)^2\left(\frac{\partial K_1}{\partial X}\right)_{\mathrm{H}}, \\ \varkappa_0 &= \varrho_{00} - \varrho_{\mathrm{F}} \cong \frac{1}{2h}(R_1 - R_0)^2\left(\frac{\partial K_0}{\partial X}\right)_{\mathrm{H}}. \end{aligned} \tag{3}$$

R_0 and R_1 are the radius vectors of the potential hypersurface minima of the ground, $E_0(R)$, and excited, $E_1(R)$, states; $K_n = \partial^2 E_n(R)/\partial R^2$ indicates the curvature of the corresponding hypersurface.

Reprint requests to Prof. Dr. O. E. Polansky, Max-Planck-Institut für Strahlenchemie, Stiftstraße 34–36, D-4330 Mülheim a.d. Ruhr.

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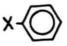
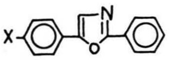
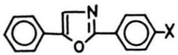
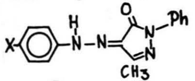
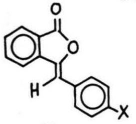
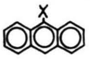
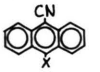
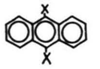
Table 1. ϱ_{00}, $\varkappa_0$ and $\varkappa_1$ values (in 10^{-3} cm^{-1}) for donor and acceptor substituents. Solvents: a) cyclohexane; b) toluene; c) ethanol; d) dioxan; e) heptane.

Compound	No.	Solv.	σ_X	ϱ_{00}	$\varkappa_0$	$\varkappa_1$	Ref.
	1	a	$\sigma < 0$ $\sigma > 0$	+ 7.23 − 3.56	− 0.04 − 1.43	− 0.38 − 0.74	[14]
	2	b	$\sigma < 0$ $\sigma > 0$	+ 4.34 − 6.00	+ 0.39 + 2.18	− 1.06 + 0.75	[15]
	3	b	$\sigma < 0$ $\sigma > 0$	+ 3.55 − 4.50	+ 0.33 − 0.05	+ 0.86 − 1.35	[15]
	4	a	$\sigma < 0$ $\sigma > 0$	+ 1.95 − 0.50	+ 3.05 + 0.60	+ 2.94 + 0.30	[8]
	5	c	$\sigma < 0$ $\sigma > 0$	+ 6.31 − 2.27	− 0.95 + 0.84	− 0.93 + 0.83	[9]
	5	d	$\sigma < 0$ $\sigma > 0$	+ 4.40 − 1.17	− 0.42 − 0.37	− 0.42 − 0.36	[9]
	6	e	$\sigma < 0$ $\sigma > 0$	+ 0.38 − 2.27	− 0.21 + 0.04	− 0.14 + 0.19	[16]
	7	e	$\sigma < 0$ $\sigma > 0$	+ 4.70 − 2.16	− 0.72 + 0.12	− 0.66 + 0.12	[16]
	8	e	$\sigma < 0$ $\sigma > 0$	+ 6.55 − 4.27	− 0.37 + 0.10	− 0.35 + 0.11	[16]

2. Results and Discussion

The experimental data are taken from eight different classes of conjugated organic compounds (see Table 1). While compounds 1, 6, 7, 8 are typically aromatic, a strong bond length alternation has to be expected in compounds 2, 3, 4, 5. The data for the classes 1—4 are quoted in [1], that for the others are calculated from the linear correlations shown in Figures 1—4. In all correlations all the data available have been used.

2.1. General Conclusions About the Linear Correlations of $\Delta\nu^{00}$, $\Delta\nu^{A}$ and $\Delta\nu^{F}$ with the σ-Hammett Constants

From the data in Figs. 2, 3, 4 [1], Figs. 1—4 in the present paper, Fig. 3 [8] and Fig. 2 [9] it can be seen that in general donor and acceptor substituents correlate separately with the σ_X's and follow (1). The only exception from those 24 correlations is for the fluorescence maxima of phenylazopyrazolone dyes — Fig. 3 [8], where a linear dependency is observed for the whole σ_X region.

In all cases investigated we looked not only for a correlation with the σ-para Hammett constants, but also for a dual substituent parameter equation with the induction σ_I and resonance σ_R-Hammett constants as well. But the correlation coefficients obtained for the dependencies of the $\Delta\nu$'s upon σ_I and σ_R are low, i.e. the separation of the two

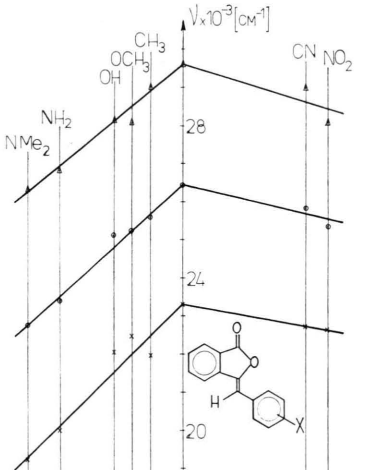


Fig. 1. Linear correlations of 0–0 transitions (⊙), absorption (△) and fluorescence (×) maxima with σ_p-Hammett constants for some substituted 3-phenyl-methylene-1(3H)-isobenzofuranones in dioxan (No. 5 in Table 1).

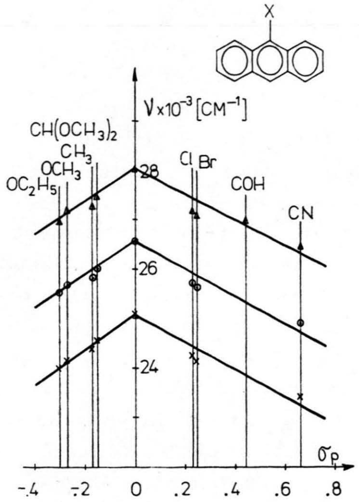


Fig. 2. Linear correlations of 0–0 transitions (⊙), absorption (△) and fluorescence (×) maxima with σ_p-Hammett constants for 9-X-antracene in heptane (No. 6 in Table 1).

effects is not pronounced. This observation is supported also by Murrell's conclusions [10], made on the basis of his studies of substituted benzenes, that the decreasing of the FC absorption transition energy as a result of substitution both with acceptors and donors indicates the nonseparability of mesomeric from inductive effects in substituted benzenes. Usually these two effects are separable from each

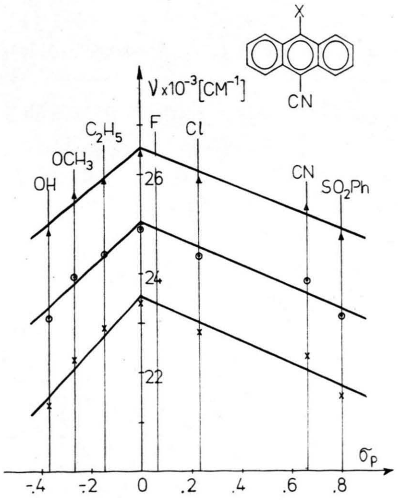


Fig. 3. Linear correlations of 0–0 transitions (⊙), absorption (△) and fluorescence (×) maxima with σ_p-Hammett constants for 9-CN,10-X-antracene in heptane (No. 7 in Table 1).

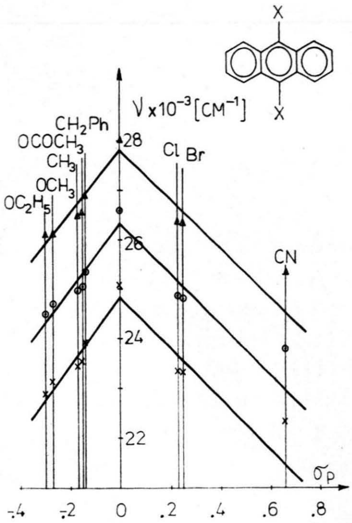


Fig. 4. Linear correlations of 0–0 transitions (⊙), absorption (△) and fluorescence (×) maxima with σ_p-Hammett constants for 9,10-di-X-antracene in heptane (No. 8 in Table 1).

other in the applications of the σ-Hammett equation [2] to equilibrium or rate constants. So its failure in the examples described above may be a consequence of principle differences between the relations (1) and the classical Hammett equation [2], where the influence of the substituent X on the reaction centre Y of the system X-M-Y is evaluated.

In spectral excitations an electronic interaction similar to that between substituent and reaction center takes place in CT excitations where some net charges flow between X and Y. And, indeed, Saidov and Bachshiev [7] have shown that the oscillator strengths of the longest wavelength CT bands, proportional to the transition densities, exhibit such a linear relation with the $|\sigma_X|$'s, but the spectral shifts do not correlate.

In contrast to that we obtain linear correlations (1) for compounds with (No. 4, 5, 7) or without (No. 1, 6, 8) a reaction centre in the molecule, as well as for systems with and without (No. 1, 6) any CT electron transitions. This unambiguously shows that correlations (1) cannot be understood in the same way as the classical Hammett dependencies [2]. This seems to be reasonable, having in mind that the approach proposed in [1] accounts for the influence of the substituent on the electronic and vibrational energies of two delocalized states, ground and excited state, and does not reflect the changes in any definite reaction centre in the molecule.

Probably for this reason the inductive effect cannot be separated from the mesomeric one in the correlations of the electron transition energies with the σ_X-Hammett constants.

2.2. Influence of the Substituents on the 0–0 Electron Transition Energies

The eight classes of organic compounds investigated differ considerably in their charge and bond-length alternation, as well as in the type of the longest wavelength electron transitions (in the sense of the MIM method [11] or Baba's configuration analysis [12]). Nevertheless, in all cases $\varrho_{00}\sigma_X < 0$ — Table 1. According to [1] this means

$$\Delta\nu_X^{00} = \nu_X^{00} - \nu_H^{00} < 0 \quad (4)$$

or

$$\nu_X^{00} < \nu_H^{00},$$

i.e. in all eight cases the energy gap between the ground and excited state decreases with substitution both with donors and acceptors. Such a dependency seems to be true for all $\pi\pi^*$ transitions. The statement above appears to be quite important for the estimation of the fluorescence ability of such classes of luminiphores, where $n\pi^*$ and $\pi\pi^*$ excited states are close. While the energy of the $n\pi^*$ level slightly depends on substitution [13], the decreasing of the $\pi\pi^*$ transition energy leads to separation of the two levels and, hence, to a considerable increase of the fluorescence quantum yield of the substituted molecule because of the smaller probability for non-radiative deactivation via the $n\pi^*$ state. In some series the fluorescence quantum yields even correlate linearly with σ-Hammett constants [9].

The lessening of the energy gap between the S_0 and S_1 states as a result of substitution can be presented as

$$h\Delta\nu_X^{00} = (E_X^1 - E_H^1) - (E_X^0 - E_H^0) < 0\,, \quad (4a)$$

where E^0 and E^1 are the energies of the minima of S_0 and S_1. The results from the quantum chemical calculations (PPP, CNDO, MINDO 3 etc.) show that substitution always leads to a decrease of the S_0 energy of the molecule, $E_H^0 > E_X^0$, and, having in mind (4a), it follows

$$|(E_X^1 - E_H^1)| > |(E_X^0 - E_H^0)| \quad \text{and}$$
$$E_X^1 - E_H^1 < 0\,. \quad (5)$$

Hence, in all classes of organic compounds investigated the influence of the substituent is greater on S_1 than on S_0. Probably, this effect is related with the higher polarizability of the excited states.

According to (2), ϱ_{00} is a measure for the change of the 0–0 electron transition energy upon substitution, and for each class of conjugated compounds ϱ_{00} has a characteristic value. From Table 1 it can be seen that the influence of the acceptor substituents on the 0–0 transition energy usually is weaker than that of the donor substituents, when the unsubstituted molecule contains acceptor groups, i.e. CN (No. 7), C=O (No. 4), COO (No. 5), or when it has even slight acceptor properties, i.e. benzene (No. 1), antracene (No. 6, 8). In such cases the substituted molecule XM could be considered as a donor–acceptor (D–A) or acceptor–acceptor (A–A) system, depending on the substituent X. One could expect that in such molecules the donor substituents will polarize the electron states (and particularly S_1) to a greater extent than the acceptors, and thus the energy gap will decrease more strongly. The weaker influence of both kinds of substituents on the ϱ_{00} of the phenylazopyrazolone dyes investigated (No. 4) is due to the π electron pair on the nitrogen atom, attached to the X-benzene ring [8]. In the XM system it is situated between the substituent X and the acceptor C=O group, X...N...C=O, and considerably decreases the transmission of the effect of the substituent upon the C=O group. In contrast to this case, the acceptors shift the 0–0 transitions in compounds 2 and 3 to a greater extent. Probably, this is connected with the two resonance structures of the oxazoles [1], which will be perturbed more by electron accepting substituents.

The comparison of the classes 6 and 8 in Table 1 shows that the introduction of a second substituent, identical with the first one and in an equivalent position of the chromophoric system, in this case 9,10-antracene, almost doubles ϱ_{00}.

One has to expect that the influence of the substituent, i.e. ϱ_{00}, decreases, with the increasing length of the conjugated systems; the comparison of No. 1 with No. 6 confirms this.

2.3. Influence of the Substituents on the Steepness of the Potential Hypersurfaces in the S_0 and S_1 States

The quantities $\varkappa_n$, defined by (3), characterize the changes in the steepness of the potential hypersurfaces $E_n(R)$ as a result of substitution X. A positive (negative) value of the product $\varkappa_n \sigma_X$ means an increase (decrease) of the steepness [1]. The data in Table 1 show that donor and acceptor substituents have a considerably different influence on the potential hypersurface steepness — this fact cannot be estimated without the analysis of the experimental data as proposed in [1]. For acceptor substituted antracene derivates, $\varkappa_n$ is approximately zero in both, the S_0 and S_1 states. As Table 1 shows, with the exception of No. 2, $\sigma < 0$, in all other cases both groups of substituents effect the force constants of ground and excited states in the same direction. The change of the solvent polarity may cause a change in the sign of $\varkappa_n \sigma_X$ (No. 5 in Table 1).

2.4. *Conditions for Bathochromic or Hypsochromic Shift of the FC Absorption and Emission Transitions*

2.4.1 Absorption

By definition

$$\Delta\nu^{A} = \nu^{A}(X) - \nu^{A}(H),$$

and in according to (1)

$$\Delta\nu^{A} = (\varrho_{00} + \varkappa_1)\,\sigma_X = \varrho_{00}\,\sigma_X + \varkappa_1\,\sigma_X . \qquad (7)$$

As shown in 2.2., for all $\pi\pi^*$ transitions there is

$$\varrho_{00}\,\sigma_X < 0$$

for both $\sigma_X > 0$ and $\sigma_X < 0$. Consequently, if $(\varkappa_1 \sigma_X) < 0$, $\Delta\nu^{A}$ will be also negative — the substituent will cause a bathochromic shift of the absorption maximum. If $(\varkappa_1 \sigma_X) > 0$, depending on $|\varkappa_1 \sigma_X|$ two cases are possible:

$$|\varkappa_1 \sigma_X| < |\varrho_{00}\,\sigma_X| \ldots (\varrho_{00}\,\sigma_X + \varkappa_1 \sigma_X) < 0\,, \qquad (8)$$

$$|\varkappa_1 \sigma_X| > |\varrho_{00}\,\sigma_X| \ldots (\varrho_{00}\,\sigma_X + \varkappa_1 \sigma_X) > 0\,. \qquad (8')$$

In the first case, (8), the decrease of the energy gap is more significant than the increase of the FC transition energy as a result of the greater steepness of the potential hypersurface in S_1 upon substitution, and this finally will lead to a bathochromic shift of the absorption maximum. In case of (8′) the substituent will cause a hypsochromic shift.

2.4.2. Fluorescence

Once again by definition

$$\Delta\nu^{F} = \nu^{F}(X) - \nu^{F}(H),$$

and according to (1)

$$\Delta\nu^{F} = (\varrho_{00} - \varkappa_0)\,\sigma_X = \varrho_{00}\,\sigma_X - \varkappa_0\,\sigma_X . \qquad (9)$$

As $(\varrho_{00}\,\sigma_X) < 0$, the increase of the steepness in the S_0 state $(\varkappa_0 \sigma_X) > 0$ will lead to a bathochromic displacement of the fluorescence maximum, $\Delta\nu^{F} < 0$. If $(\varkappa_0 \sigma_X) < 0$, a bathochromic shift will be observed when $|\varrho_{00}\,\sigma_X| > |\varkappa_0 \sigma_X|$, and a hypsochromic one when $|\varrho_{00}\,\sigma_X| < |\varkappa_0 \sigma_X|$. For illustration two typical cases, presented in Table 1, will be considered. For comparability of the numerical results we shall use $|\sigma_X| = 1$, i.e. $\sigma_X = -1$ for donor and $\sigma_X = 1$ for acceptor substituents.

(i) Class No. 1 (Table 1):

The substituents have a greater influence on the energy gap, than on the steepness of the hypersurfaces in S_0 and S_1. From the experimental data and (7) follows

$$\Delta\nu^{A} = -6850\ \text{cm}^{-1} = -7230 + 380 \quad \text{for} \quad \sigma_X = -1\,,$$

$$\Delta\nu^{A} = -4300\ \text{cm}^{-1} = -3560 - 740 \quad \text{for} \quad \sigma_X = +1\,.$$

The absorption spectra move strongly to the red and according to (7) this effect is mainly due to the lessening of the energy gap. In this case the donors increase, while the acceptors decrease the steepness of the S_1 potential hypersurface. For the fluorescence maxima shifts:

$$\Delta\nu^{F} = -7270\ \text{cm}^{-1} = -7230 - 40 \quad \text{for} \quad \sigma_X = -1\,,$$

$$\Delta\nu^{F} = -2160\ \text{cm}^{-1} = -3560 + 1400 \quad \text{for} \quad \sigma_X = +1\,.$$

The strong bathochromic displacement observed for $\sigma_X < 0$ results entirely from the decrease of the 0–0 transition energy (see (9)).

Acceptor substituents cause a weaker bathochromic shift of the fluorescence maxima, because the decrease of the steepness of S_0 to a considerable extent compensates the lessening of the energy gap.

(ii) Class No. 4 (Table 1):

The influence of the substituents on ϱ_{00} is weaker and commensurable with that on $\varkappa_0$ and $\varkappa_1$. According to (7)

$$\Delta\nu^{\mathrm{A}} = -4900\ \mathrm{cm}^{-1} = -1950 - 2950 \quad \text{for} \quad \sigma_X = -1\,,$$

$$\Delta\nu^{\mathrm{A}} = -200\ \mathrm{cm}^{-1} = -500 + 300 \quad \text{for} \quad \sigma_X = +1\,.$$

The strong effect of the donor substituents on $\Delta\nu^{\mathrm{A}}$ results mainly from the decrease of the steepness of S_1, and to a smaller extent from the lessening of the energy gap. Due to the almost complete compensation of the two effects [9], the acceptor substituents cause an unsignificant bathochromic shift of the absorption maxima.

From (9) results

$$\Delta\nu^{\mathrm{F}} = 1100\ \mathrm{cm}^{-1} = -1950 + 3050 \quad \text{for} \quad \sigma_X = -1\,,$$

$$\Delta\nu^{\mathrm{F}} = -1100\ \mathrm{cm}^{-1} = -500 - 600 \quad \text{for} \quad \sigma_X = +1\,.$$

In this case the donors cause a large decrease of the hypersurface steepness in the S_0 state, which dominates over the lessening of the energy gap, and a hypsochromic shift of the fluorescence maxima is observed. For $\sigma_X > 0$ the two effects have the same sign, causing red shift of the fluorescence maxima.

2.5. Influence of the Substituents on the Stokes Shift

The Stokes shifts for the substituted (XM) and the unsubstituted (HM) molecules can be denoted by

$$\Delta\nu^{\mathrm{St}}(\mathrm{X}) = \nu^{\mathrm{A}}(\mathrm{X}) - \nu^{\mathrm{F}}(\mathrm{X})\,,$$

$$\Delta\nu^{\mathrm{St}}(\mathrm{H}) = \nu^{\mathrm{A}}(\mathrm{H}) - \nu^{\mathrm{F}}(\mathrm{H})\,.$$

Then, the influence of the substituent X on the Stokes loss $\Delta(\Delta\nu^{\mathrm{St}})$ can be presented as

$$\begin{aligned}\Delta(\Delta\nu^{\mathrm{St}}) &= \Delta\nu^{\mathrm{St}}(\mathrm{X}) - \Delta\nu^{\mathrm{St}}(\mathrm{H})\\ &= ((\nu^{\mathrm{A}}(\mathrm{X}) - \nu^{\mathrm{F}}(\mathrm{X}))\\ &\quad - (\nu^{\mathrm{A}}(\mathrm{H}) - \nu^{\mathrm{F}}(\mathrm{H})))\\ &= ((\nu^{\mathrm{A}}(\mathrm{X}) - \nu^{\mathrm{A}}(\mathrm{H}))\\ &\quad - (\nu^{\mathrm{F}}(\mathrm{X}) - \nu^{\mathrm{F}}(\mathrm{H})))\\ &= \Delta\nu^{\mathrm{A}} - \Delta\nu^{\mathrm{F}} = \varrho_{\mathrm{A}}\,\sigma_X - \varrho_{\mathrm{F}}\,\sigma_X\\ &= (\varkappa_1 + \varkappa_0)\,\sigma_X\,. \qquad (10)\end{aligned}$$

It follows from the analysis of the data in Table 1 that for compounds No. 2, 5–8 the increase of $\Delta(\Delta\nu^{\mathrm{St}})$ results from the simultaneous increase of the steepness of the S_0 and S_1 hypersurfaces. In compounds No. 1, 4 the donor and acceptor substituents cause opposite changes in the steepness of the S_0 and S_1 hypersurfaces, and this leads to a different substituent effect on the $\Delta(\Delta\nu^{\mathrm{St}})$ values.

3. Conclusion

The discussion above demonstrates the usefullness of the analysis of experimental results by the approach proposed in [1], which allows to understand both equally and oppositely directed shifts of the maxima of absorption and fluorescence, respectively. Even more important is that in this approach [1] the experimental shifts are described as a result of two independent contributions, the one due to a change in the energy gap, the other due to the change in the force constants.

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