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On the validity of the constants of ionic substituents. Substituent effects on the cyano stretching frequencies and intensities of *trans*-α-phenyl-β-arylacrylonitriles

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Abstract

Fourier-transform IR frequencies ν(C≡N) and integrated intensities A(C≡N) of the cyano groups of a series of *trans*-α-phenyl-β-arylacrylonitriles (51 compounds) have been measured. Both ν(C≡N) and the square roots of A(C≡N) of the neutral m- and p-substituted compounds (34 examples) have been found to correlate satisfactorily with σ^+ substituent constants, as well as according to the equation of Yukawa-Tsuno. Diortho-substituted compounds deviate strongly from the correlation lines because of the steric ortho-effects mainly. σ^+ (and other) constants of ionic substituents (seven examples) have proved satisfactorily valid in the series studied. The transmission coefficient of the C=C double bond in the series has been estimated to be 0.7.

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1. Introduction

There is a discussion in the literature on the validity of the constants of ionic [1] (unipolar [2–4], charged [5,6]) substituents. It has recently been mentioned by Hansch et al. [2] and reviewed in detail by Shorter [3]. The discussion was opened by Jaffe in 1953 [1]; it was intensified in 1978 by Wepster and his colleagues [7]. The most conflicting opinions are given here.

(i) "Changed substituents cannot be included with dipolar groups in one general scale of electronic substituent effects" [6] "Such values would only be valid for a particular geometry and the method of measurement employed." [6].

(ii) σ^+ and other constants of anionic substituents (determined on the basis of cyano IR frequencies and intensities [8]), like the constants of neutral [1] (dipolar [2–4]) substituents, "can be used as an approximate quantitative measure of the electronic effects of anionic substituents in other spectroscopic and (maybe) chemical series." [9]

The first statment is based on electrostatic calculations and it is illustrated by literature examples [6]; the second one has purely empirical support [10]. The above opinions are very distant, but not fully contrary, since all the tested examples [9,10] are similar in geometry, and their geometry is similar to that of the definition series (benzonitriles): the distances between the substituent R and the indicator group X are close (I, where R are various substituents in m- and p-positions; 276 compounds in all, of which 54 have anionic substituents R [8–10]).

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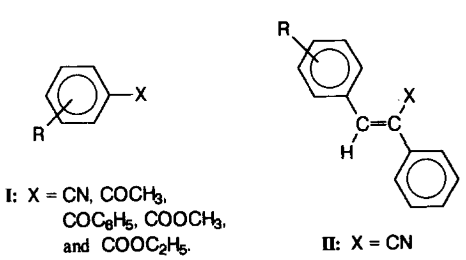

Scheme 1.

trans-α-Phenyl-β-arylacrylonitriles (**II**) have quite a different geometry, especially the distance between R and X (considered as points) in **II** is longer that in **I** (about 1.3 and 1.1 times for meta-s-trans- and para-substituted compounds respectively). Thus we hope a study of these compounds will make it possible to check the above statement (i), especially about the importance of the geometric factor.

2. Experimental

Most of the compounds studied were available from previous investigations [11]. Others were prepared and purified according to the literature. *Trans*-α-phenyl-β-4-methylthiophenylacrylonitrile was perpared as follows: a solution of 1.5 g of 4-(methylthio)benzaldehyde and 1.2 g of phenylacetonitrile in 15 ml of dry ethanol was made alkaline by adding a few drops of sodium ethoxide in dry ethanol and standing for 2 h at room temperature. The crystals were filtered-off, washed with ethanol and recrystallized from ethanol. Colourless crystals (1.9 g) were obtained: m.p. 96°C. For $C_{15}H_{13}NS$ (251.35) (element, % calcd., % found): C, 76.46, 76.53; H, 5.21, 5.03; N, 5.57, 5.45; S, 12.76, 12.88. *trans*-α-phenyl-β-4-trimethylammoniophenylacrylonitrile iodide was prepared by a 3 week standing at room temperature of a solution of 2.9 g of *trans*-α-phenyl-β-4-trimethylaminophenylacrylonitrile (m.p. 134°C, obtained from 4-(dimethylamino)benzaldehyde and phenylacetonitrile, as above) and 8 ml (strong excess) of methyl iodide in 75 ml of benzene. The crystals were filtered-off and washed three times with benzene. Pale yellow, fine crystals (1.0 g) were obtained: m.p. 190°C, with decomposition (gas evolution). For $C_{18}H_{19}IN_2$ (390.29) (element, % calcd, % found): C, 55.39, 55.70; H, 4.92, 5.19; N, 7.18, 7.13.

Anions (*trans*-α-phenyl-β-arylacrylonitriles with anionic substituents) were prepared by reacting the solutions of the corresponding N–H and O–H conjugate acids with dry sodium methoxide under argon; their spectra were recorded immediately. The bands of the parent conjugate acids must not be present in these spectra.

Spectra of 0.05–0.1 mol l^{-1} dimethyl sulphoxide (DMSO) solutions of all the compounds studied were recorded using a Bruker 113v FT IR spectrometer, in CaF_2 cells. The complex band of *trans*-α-phenyl-β-4-cyanophenylacrylonitrile was decomposed into α-CN and p-CN components.

3. Statistics

Most of the σ and σ^+ constants, used for m- and p-substituents (Table 1A), have been taken from the review [2]; σ^+ of the aza-substituents have been taken from Ref. [12], and their σ values from the book in Ref. [5] (mean values). $\sigma^+_m = \sigma_m$ has been assumed for the missing values of the meta-substituents HO, CH_3O, H_2N, F, Cl, Br and O_2N. The σ^0 values have been taken from the book in Ref. [4]; $\sigma^0_m = \sigma_m$ has been assumed for *m*-CH_3CONH and *m*-aza; $\Delta\sigma^+_R = \sigma^+ - \sigma^0$ have been calculated in all cases; an additive scheme was used for the m- and p-polysubstituted compounds. The mean values of σ^+, given in Ref. [5], have been used for the ortho-substituted heteroaryls and polycyclic

Table 1
Infrared data (solvent DMSO) for *trans*-α-phenyl-β-arylacrylonitriles: $R_nC_6H_{5-n}$–CH=CH(C_6H_5)C≡N

No.	Substituent (R)	ν(C≡N) (cm^{-1})	A(C≡N) ($km\ mol^{-1}$)	$A^{1/2}$(C≡N)	σ	σ^+	σ^0	σ_R^+
A. m- *and* p-*substitued compounds*								
1.	H	2214.4	18.75	4.33	0	0	0	0
2.	3-CH_3	2212.0	21.43	4.63	−0.07	−0.13	−0.07	−0.06
3.	4-CH_3	2213.9	22.56	4.75	−0.17	−0.31	−0.12	−0.19
4.	4-$(CH_3)_2CH$	2212.9	21.30	4.62	−0.15	−0.28	−0.16	−0.12
5.	4-C_6H_5	2212.7	21.39	4.62	−0.01	−0.18	0.04	−0.22
6.	3,4-$(CH)_4$ [a]	2212.0	20.91	4.57	−0.05	−0.27	–	–
7.	3-HO	2213.9	18.06	4.25	0.12	0.12	0.04	0.08
8.	4-HO	2208.1	32.49	5.70	−0.37	−0.92	−0.13	−0.79
9.	3-CH_3O	2213.9	19.27	4.39	0.12	0.12	0.06	0.06
10.	4-CH_3O	2210.1	34.57	5.88	−0.27	−0.78	−0.16	−0.62
11.	3,4-$(CH_3O)_2$	2209.1	27.59	5.25	−0.15	−0.66	−0.10	−0.56
12.	3,5-$(CH_3O)_2$	2213.2	20.09	4.48	0.24	0.24	0.12	0.12
13.	2,4,5-$(CH_3O)_3$	2209.1	26.10	5.11	−0.03	−0.56	−0.04	−0.50
14.	3-C_2H_5O-4-CH_3O	2208.1	28.06	5.30	−0.17	−0.68	−0.10	−0.58
15.	3,4-CH_2O_2 [b]	2210.1	25.57	5.06	−0.16	−0.68	−0.16	−0.52
16.	3-H_2N	2212.0	22.37	4.73	−0.16	0.16	−0.14	−0.02
17.	4-H_2N	2199.4	52.71	7.26	−0.86	−1.30	−0.38	−0.92
18.	4-CH_3NH	2200.4	54.91	7.41	−0.70	−1.81	−0.40	−1.41
19.	4-$(CH_3)_2N$	2202.3	52.27	7.23	−0.83	−1.70	−0.44	−1.26
20.	3-CH_3CONH	2212.9	19.18	4.38	0.21	0.21	0.21	0
21.	4-CH_3CONH	2210.1	28.30	5.32	0.00	−0.60	0.03	−0.57
22.	3-C_6H_5CONH	2213.4	17.51	4.18	0.02	0.02	0.02	0
23.	4-CH_3S	2211.1	23.24	4.82	0.00	−0.60	0.08	−0.52
24.	3-F	2214.1	17.06	4.13	0.34	0.34	0.35	−0.01
25.	3-Cl	2215.8	14.06	3.75	0.37	0.37	0.37	0
26.	4-Cl	2214.4	17.31	4.16	0.23	0.11	0.27	−0.16
27.	3-Br	2215.4	13.76	3.71	0.32	0.39	0.38	−0.01
28.	4-Br	2214.1	17.56	4.19	0.48	0.15	0.26	−0.11
29.	4-COOH	2216.3	12.46	3.53	0.45	0.42	–	–
30.	4-CN [c]	2217.4	[j]	[j]	0.66	0.66	0.69	−0.03
31.	3-NO_2	2216.6	12.39	3.52	0.71	0.71	0.71	0.01
32.	4-NO_2	2217.8	11.83	3.44	0.78	0.79	0.82	−0.03
33.	3-aza [d]	2216.0	13.82	3.72	0.62	0.30	0.62	−0.32
34.	4-aza [e]	2218.0	9.80	3.13	0.88	0.86	–	–
B. o-*Substituted compounds* [f]								
35.	2,4,6-$(CH_3)_3$	2218.7	13.46	3.67	–	−0.93		
36.	2,3-$(CH)_4$ [g]	2215.8	17.29	4.16	–	−0.44		
37.	2,3,5,6-C_8H_8 [h]	2219.7	6.86	2.62	–	−0.97		
38.	2,3,4$C_{10}H_7$ [i]	2213.9	23.47	4.84	–	−0.81		
39.	2,6-$(CH_3O)_2$	2218.7	11.22	3.35	–	0.22		
40.	2,6-$(Cl)_2$	2223.6	7.18	2.68	–	−1.56		
41.	2-Br	2218.7	13.09	3.62	–	0.15		
42.	2-NO_2	2219.7	12.21	3.49	–	0.79		
43.	2,3-oxa [k]	2212.0	27.05	5.20	0.61	−0.89		
44.	2,3-thia [l]	2207.2	17.25	4.14	0.41	−0.78		
C. Positive and negative ions								
45.	4-$(CH_3)_3N^+(I^-)$	2216.0	13.69	3.70	0.60	0.41	0.80	−0.39
46.	3-$O^-(Na^+)$	2208.1	26.94	5.19	−0.47	−1.15	−1.38	0.23
47.	4-$O^-(Na^+)$	2187.9	112.78	10.6	−0.81	−4.27	−2.67	−1.59
48.	3-$CH_3CON^-(Na^+)$	2211.0	23.23	4.82	–	−0.75	−0.93	0.18
49.	4-$CH_3CON^-(Na^+)$	2198.5	73.10	8.55	–	−2.90	−0.96	−1.92
50.	3-$C_6H_5CON^-(Na^+)$	2209.6	22.15	4.70	–	−0.38 [m]	–	–
51.	4-$CO_2^-(Na^+)$	2213.9	20.16	4.49	0.00	−0.41	−0.16	−0.25

[a] 2-Naphthyl derivative; [b] methylenedioxy substituent; [c] data for the α-cyano group, see Experimental Section; [d] 3-pyridyl derivative; [e] 4-pyridyl derivative; [f] not included into the statistical treatments; [g] 1-naphthyl derivative; [h] 9-anthryl derivative; [i] 1-pyrenyl derivative; [j] no reliable data; [k] 2-furyl derivative; [l] 2-thienyl derivative; [m] our unpublished data.

aryls; the corresponding σ_p^+ values have been used for H_3C, Br and O_2N ortho-substituents (Table 1B). All the constants of anionic substituents (Table 1C) have been taken from Ref. [8].

The statistical treatment according to the equations of Hammett (1) and Brown–Okamoto (2)

$$y = \rho\sigma + b \tag{1}$$

$$y = \rho\sigma^+ + b \tag{2}$$

has been performed by using a standard programme for single-parameter linear regressions. The treatment according to the equation of Yukava–Tsuno (3)

$$y = \rho(\sigma^0 + r^+\Delta\sigma_R^+) + b \tag{3}$$

was carried out by a standard programme for dual-parameter linear regressions using the mathematically equivalent equation (4)

$$y = \rho\sigma^0 + \rho^+\Delta\sigma_R^+ + b \tag{4}$$

with a posterior calculation of $r^+ = \rho^+/\rho$ (cf. Eqs. (3) and (4)).

4. Results and discussion

The frequencies $\nu(C{\equiv}N)$ and integrated intensities $A(C{\equiv}N)$ of the cyano stretching bands of the *trans*-α-phenyl-β-arylacrylonitriles studied are listed in Table 1 together with the corresponding substituent constants. DMSO, a polar aprotic solvent, has been chosen for this study, for it dissolves equally well both the neutral compounds and ions studied, and does not react with them. The results of the statistical treatment of both $\nu(C{\equiv}N)$ and $A^{1/2}(C{\equiv}N)$ correlations with substituent constants (see Statistics Section) are included in Table 2; the graphical comparison of these values is shown on Figs. 1 and 2. The correlations with σ are much poorer (R values of 0.89 for $\nu(C{\equiv}N)$ and 0.82 for $A^{1/2}(C{\equiv}N)$); they cannot be used for any practical purpose, so they are not included in Table 2.

4.1. *Meta- and para-substituted compounds*

The correlations of both $\nu(C{\equiv}N)$ and $A^{1/2}(C{\equiv}N)$ of these compounds have already been studied for chloroform as solvent [11]. Values of ρ and R of the $\nu(C{\equiv}N)/\sigma^+$ correlations for DMSO are somewhat higher than those for $CHCl_3$; the opposite rule is valid for the $A^{1/2}(C{\equiv}N)/\sigma^+$ correlations (data from Ref. [11b], recalculated for $A(C{\equiv}N)$ in km mol^{-1}). The transmission coefficient $\pi = \rho(\text{bridged})/\rho(\text{unbridged})$ of the C=C double bond can be estimated on the basis of the present data (reference series: benzonitriles, data for the corresponding solvent [8b]) at 0.66 (for $\nu(C{\equiv}N)$) and 0.67 (for $A^{1/2}(C{\equiv}N)$). We have calculated for comparison: (a) the same series, solvent $CHCl_3$ [11b]: 0.55 and 0.86, respectively; (b) p-substituted *trans*-cinnamonitriles, solvent CCl_4: 0.83 and 0.61 (on the basis of Butt and Topsom's data [13]); (c) substituted benzylidene malononitriles, solvent $CHCl_3$ [14]: 0.49. A discussion on the influence of both electronic and geometrical factors on the transmission coefficient of the C=C bridge has already been published for nitriles [14] and ketones [15].

The amino-substituted compound deviates from both the $\nu(C{\equiv}N)/\sigma^+$ (strongly, -6.2 cm^{-1}) and $A^{1/2}(C{\equiv}N)/\sigma^+$ (not so strongly) correlation lines (Figs. 1 and 2). These derivations are probably due to some specific interaction of the amino group with a polar aprotic solvent (DMSO). A similar result (a mean $\nu(C{\equiv}N)$ deviation of -10.8 cm^{-1}) has been found in the benzonitrile series for DMSO and hexamethylphosphoric triamide as solvents [8].

Table 2

Correlations of frequencies $\nu(C\equiv N)$ and square roots of intensities $A^{1/2}(C\equiv N)$ ($A(C\equiv N)$ in km mol^{-1}) of the cyano groups of *trans*-α-phenyl-β-arylacrylonitriles with substituent constants, according to the equations of Brown–Okamoto (Eq. (2)) and Yukawa–Tsuno (Eq. (3))

No.	Series	Sigma	Slope	b [a]	R [b]	s.d. [c]	n [d]
A. Correlation of $\nu(C\equiv N)$							
1.	Neutral compounds	σ^+	$\rho = 6.02$	2213.3	0.9682	1.00	33 [e]
2.	Neutral	$\sigma^0, \Delta\sigma_R^+$	$\rho = 5.42, r^+ = 1.22$	2213.4	0.9689	1.00	30 [f]
3.	Ions	σ^+	$\rho = 6.06$	2214.9	0.9927	1.31	7
4.	Ions	$\sigma^0, \Delta\sigma_R^+$	$\rho = 6.12, r^+ = 1.01$	2215.2	0.9940	1.51	6
5.	Neutral and ions	σ^+	$\rho = 5.76$	2213.5	0.9804	1.15	40 [g]
6.	Neutral and ions	$\sigma^0, \Delta\sigma_R^+$	$\rho = 5.32, r^+ = 1.20$	2213.6	0.9812	1.17	36 [h]
B. Correlation of $A^{1/2}(C\equiv N)$							
7.	Neutral compounds	σ^+	$\rho = -1.50$	4.39	0.9750	0.21	32
8.	Neutral compounds	$\sigma^0, \Delta\sigma_R^+$	$\rho = -1.43, r^+ = 1.08$	4.40	0.9772	0.21	29 [i]
9.	Ions	σ^+	$\rho = -1.56$	3.83	0.9929	0.34	7
10.	Ions	$\sigma^0, \Delta\sigma_R^+$	$\rho = -1.35, r^+ = 1.38$	3.88	0.9984	0.20	6
11.	Neutral and ions	σ^+	$\rho = -1.46$	4.33	0.0795	0.29	40
12.	Neutral and ions	$\sigma^0, \Delta\sigma_R^+$	$\rho = -1.22, r^+ = 1.41$	4.29	0.9867	0.24	35 [c]

[a] Intercept; [b] correlation coefficient, $0 \leqslant R \leqslant 1$; [c] standard deviation; [d] number of data points; [e] point of No. 17 was excluded, which lowered R to 0.9424; [f] we did not find σ^0 for points 6, 29 and 34. Point No. 17 was excluded, which lowered R to 0.96; [g] excluding point 17; $R = 0.96$ for the whole series; [h] see footnote f; $R = 0.97$ for whole series; [i] no σ^0 data for points 6, 29 and 34.

The important result obtained, however, is that (according to Jaffe's criterion [1]) all the correlations for $\nu(C\equiv N)$ and $A^{1/2}(C\equiv N)$, are *satisfactory* (Table 2), so that they can be used for checking the validity of the constants of ionic substituents.

4.2. Ortho-substituted compounds

The Hammett-type equations are usually not obeyed for ortho-substituted compounds [5]. In certain cases, however, the correlations found are not poor: for example we have calculated on the basis of literature data [16] for series of ortho-substituted benzonitriles (solvent CCl_4, infinite dilution) that $\nu(C\equiv N)$ correlates fairly ($R = 0.94$, substituent

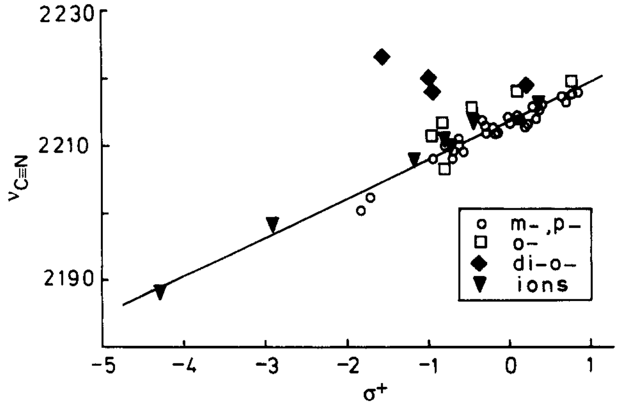

Fig. 1. Plot of $\nu(C\equiv N)$ (cm^{-1}) of *trans*-α-phenyl-β-arylacrylonitriles vs. σ^+ substituent constants.

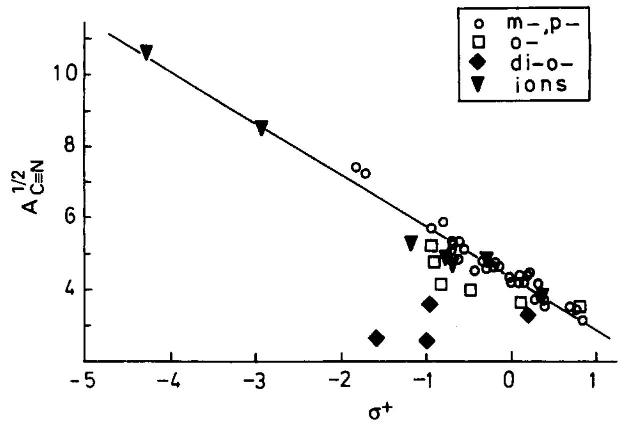

Fig. 2. Plot of $A^{1/2}(C\equiv N)$ ($A(C\equiv N)$ in km mol^{-1}) of *trans*-α-phenyl-β-arylacrylonitriles vs. σ^+ substituent constants.

ortho-F excluded), and $A^{1/2}(C\equiv N)$ correlates satisfactorily ($R = 0.97$) with σ_p^+ substituent constants (we did not find anywhere σ_0^+ constants). As seen in Figs. 1 and 2, the ortho-substituted compounds (white square points) do deviate from the correlation lines, but the strong deviations are characteristic for the di-ortho-substituted compounds (black square points). A possible explanation of this result is the following: there *is* a conformation of the mono-ortho-substituted compounds, in which the molecule is not strongly deplanarized; there is no such conformation for the di-ortho-substituted ones. Hence, we can say that for the series studied the steric factor proves to be more essential that the purely electronic ortho-effect.

4.3. Positive and negative ions

The conversion of nitriles into anions is usually accompanied by essential changes in their IR spectra [17]. Here are two examples from the present series:

(i) For *trans*-α-phenyl-β-4-hydroxyphenylacrylonitrile and its anion: downward shift and strong intensification of the ν(C≡N) band; strong intensification of the aromatic skeletal bands near 1600 cm^{-1} and near 1500 cm^{-1} of the β-phenyl ring (Fig. 3, in accordance with the work in Ref. [10b]), etc.

(ii) For *trans*-α-phenyl-β-4-acetylaminophenylacrylonitrile and its anion: downward shift and intensification of the ν(C≡N) band; about 200 cm^{-1} downward shift of the ν(C=O) band at 1690 cm^{-1}; strong intensification of the aromatic skeletal bands of the β-phenyl ring (Fig. 4), etc.

All the correlations for the ions themselves are excellent (Table 2, series 3, 4, 9 and 10), hence the constants of ionic substituents are well self-consistent. The main question, stated in the Introduction, is whether in our case the constants of the ionic substituents

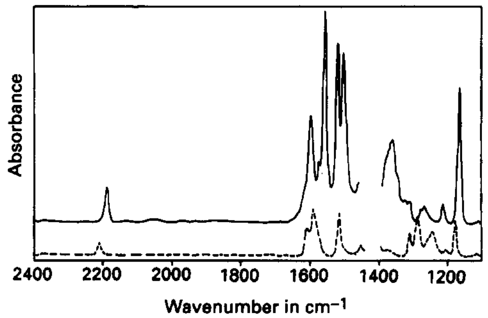

Fig. 3. IR spectrum (solvent DMSO) of *trans*-α-phenyl-β-hydroxyphenyacrylonitrile (broken line) and its anion (full line).

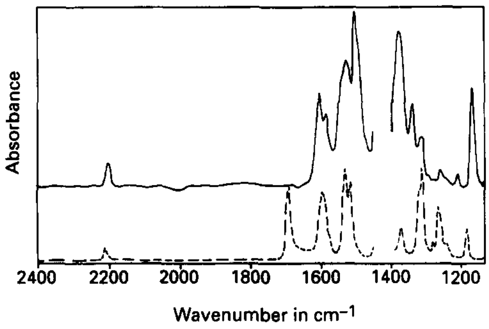

Fig. 4. IR spectrum (solvent DMSO) of *trans*-α-phenyl-β-acetylaminophenylacrylonitrile (broken line) and its anion (full line).

are consistent with those of the neutral ones. We believe the answer of this question is evident from Table 2: adding the points of the ionic substituents (Table 2, series 5, 6, 11 and 12) to the correlations of the netural compounds (Table 2, series 1, 2, 7 and 8) does not deteriorate the correlation factors. Hence, the constants of ionic substituents prove satisfactorily valid, i.e. the influence of the geometric electrostatic factor (see Introduction) proves not to be important in the series studied.

5. Conclusions

The present results provide additional support to the general known statement: linear free energy relationships (LFER) can be applied even in cases when, according to theory, they are expected not to be valid.

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