THE C=O STRETCHING VIBRATION OF AROMARIC α,β-UNSATURATED CARBONYL AND ARYLFURANCARBONYL COMPOUNDS*

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Wavenumbers of the C=O stretching fundamental in the series of 145 conformers of aromatic α,β-unsaturated carbonyl and arylfurancarbonyl compounds were investigated in terms of Yukawa–Tsuno structure-reactivity equation. The parameters of these correlations were compared with the results obtained using Hammett or Brown equation. The separation and the transmission of "normal" and resonance substituent effects have been discussed in the individual series.

Thus far only a litle attention has been given to the application of two-parameter structure-reactivity correlations in series of the C=O stretching fundamental frequencies of α,β-unsaturated carbonyl compounds. The influence of substituents on wavenumber of the C=O stretching vibration in series of substituted chalcones were investigated in terms of Taft–Ehrenson[1] and Swain–Lupton equation[2,3]. McDonald suggested[4] the application of the Yukawa–Tsuno equation to the C=O stretching fundamental of some α,β-unsaturated carbonyl compounds investigated by us previously[5] using Hammett or Brown equation. In the preceding work[5] we have employed the Yukawa–Tsuno equation to investigate the substituent effect in series of aromatic aldehydes, carboxylic acids, esters, and ketones.

Continuing our previous research in structure-reactivity relationships and taking into consideration McDonald's proposal[4], we have submitted the wavenumbers of some available series of α,β-unsaturated carbonyl and arylfurancarbonyl compounds to the correlation according to Yukawa–Tsuno equation[6,7] (Eq. (*1*)).

$$\nu = \nu^0 + \varrho(\sigma^n + r^+ \Delta\sigma_R^+)\,, \qquad (1)$$

where

$$\Delta\sigma_R^+ = \sigma^+ - \sigma^n\,.$$

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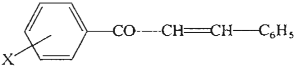
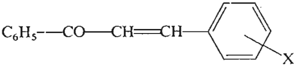
* Part II in the series Application of the Yukawa–Tsuno Equation to the Wavenumbers of the C=O Stretching Vibration; Part I: Acta Fac. Rerum Nat. Univ. Comenianae, in press.

The following disubstituted propenones were investigated: 1-aryl-3-phenyl (*I*), 1-phenyl-3-aryl (*II*), 1-phenyl-3-(5-aryl-2-furyl) (*III*), 1-phenyl-3-(5-aryl-2-thienyl) (*IV*), 1-[5-(4-chlorophenyl)-2-furyl]-3-aryl (*V*), 1-[5-(4-nitrophenyl)-2-furyl]-3-aryl



I



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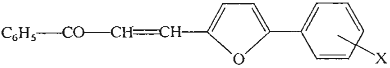

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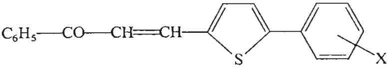

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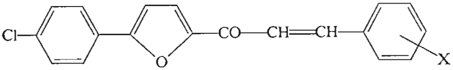

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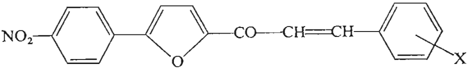

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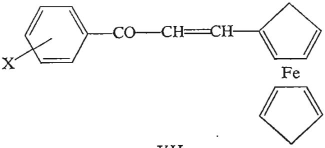
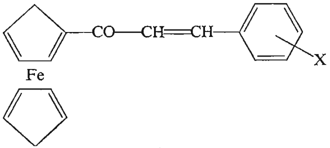
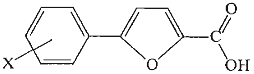


VII



VIII



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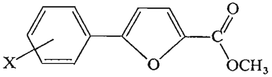


X

(*VI*), 1-aryl-3-ferrocenyl (*VII*), 1-ferrocenyl-3-aryl (*VIII*), and 5-aryl-2-furancarboxylic acids (*IX*) and their methyl esters (*X*). Similarly to the previous investigation[8] the parameters of Yukawa–Tsuno equation were compared with the corresponding results using Hammett or Brown equation, Eqs (*2*) or (*3*) resp.

$$\nu = \nu^0 + \varrho\sigma\,, \tag{2}$$

$$\nu = \nu^0 + \varrho\sigma^+\,. \tag{3}$$

EXPERIMENTAL

The Yukawa–Tsuno correlations were treated on a Siemens 4004/150 computer. The regression parameters of Hammett and Brown equations were calculated on a Hewlet–Packard 910 B calculator. The published substituent constants σ^n, σ, and σ^+ were used[9–11].

RESULTS AND DISCUSSION

Wavenumbers of the C=O stretching vibration of s-*cis* and s-*trans* conformers of aromatic α,β-unsaturated carbonyl compounds *I*–*VIII* and *cis*-O—O and *trans*-O—O conformers of arylfurancarbonyl compounds *IX*, *X* measured in CCl_4 were taken from [5,12–15] and are listed in Table I. The results of statistical treatment of data according to Eqs ((*1*)–(*3*)) are given in Table II.

TABLE I

Wavenumbers of the Stretching Fundamental (ν(C=O)) Measured in Tetrachloromethane for Series of Compounds *I*—*X* (in cm^{-1})

Compound	X	*s-cis*	*s-trans*
Series *I*			
1	4-NO_2	1 675·5	1 660·0
2	3-NO_2	1 677·5	1 659·0
3	3-Br	1 674·0	1 656·0
4	3-Cl	1 674·0	1 656·0
5	4-Br	1 672·0	1 653·5
6	4-Cl	1 672·0	1 653·5
7	3-OCH_3	1 671·0	1 655·0
8	4-F	1 673·0	1 654·0
9	H	1 671·5	1 651·5
10	4-CH_3	1 669·0	1 650·0
11	4-OCH_3	1 667·0	1 649·0
12	4-$N(CH_3)_2$	1 661·5	1 642·0
Series *II*			
13	3-NO_2	1 678·0	1 660·0
14	4-CN	1 676·0	1 658·0
15	3-Cl	1 676·0	1 657·0
16	4-Cl	1 675·0	1 653·5
17	4-F	1 674·0	1 653·5
18	H	1 671·5	1 653·5
19	4-CH_3	1 670·5	1 650·5
20	4-OCH_3	1 668·5	1 648·5
21	4-NH_2	1 667·0	1 645·0
22	4-$N(CH_3)_2$	1 663·0	1 641·5
Series *III*			
23	4-NO_2	1 671·5	—
24	3-NO_2	1 670·5	1 649·0
25	3-Br	1 670·0	1 648·0
26	3-Cl	1 669·5	1 647·0
27	4-Br	1 669·0	1 647·0
28	4-Cl	1 668·5	1 646·0
29	H	1 668·5	1 645·5
30	4-CH_3	1 667·5	1 644·5
31	4-OCH_3	1 666·0	1 642·0
Series *IV*			
32	4-NO_2	1 668·0	1 649·5
33	3-Cl	1 667·5	1 648·0
34	4-Br	1 667·0	1 647·5
35	4-Cl	1 666·5	1 647·0
36	H	1 666·0	1 647·0
37	3-CH_3	1 666·0	1 647·0
38	4-CH_3	1 665·0	1 646·0
39	4-OCH_3	1 664·5	1 645·0
Series *V*			
40	2-NO_2	1 662·0	—
41	4-NO_2	1 662·0	—
42	2-Br	1 659·0	—
43	3-OCH_3	1 659·0	—
44	2-Cl	1 660·0	—
45	4-Cl	1 660·0	—
46	H	1 658·0	—
47	2-F	1 659·0	—
48	4-F	1 659·0	—
49	4-CH_3	1 657·0	—
50	2-OCH_3	1 656·0	—
51	4-OCH_3	1 655·0	—
52	4-$N(CH_3)_2$	1 647·0	—
Series *VI*			
53	4-NO_2	1 664·0	1 643·0
54	3-NO_2	1 663·0	1 643·0
55	2-Br	1 660·0	1 641·0
56	2-Cl	1 662·0	1 642·0
57	4-Cl	1 662·0	1 641·0
58	H	1 659·0	1 641·0
59	3-CH_3	1 660·0	1 641·0
60	2-F	1 660·0	1 641·0
61	4-F	1 660·0	1 641·0
62	4-CH_3	1 658·0	1 640·0
63	4-OCH_3	1 657·0	1 640·0

TABLE I
(*Continued*)

Compound	X	*s-cis*	*s-trans*
Series *VII*			
64	4-NO_2	1 665·6	1 646·0
65	3-NO_2	1 666·0	1 645·0
66	4-CN	1 666·5	1 645·0
67	4-Br	1 665·0	1 643·0
68	3-Cl	1 664·5	1 643·0
69	4-Br	1 663·0	1 643·0
70	4-Cl	1 663·5	1 642·0
71	3-OCH_3	1 662·0	1 639·0
72	4-CH_3	1 662·5	1 638·0
73	4-OCH_3	1 660·5	1 637·0
74	4-$N(CH_3)_2$	1 657·0	1 633·0

Compound	X	*s-cis*	*s-trans*
Series *VIII*			
75	4-NO_2	1 662·5	—
76	3-NO_2	1 662·5	—
77	4-CN	1 662·0	—
78	3-Cl	1 662·0	—
79	4-Cl	1 661·0	—
80	4-F	1 660·5	—
81	H	1 660·0	—
82	4-CH_3	1 658·5	—
83	4-OCH_3	1 658·0	—
84	4-NH_2	1 657·5	—
85	4-$N(CH_3)_2$	1 656·0	—

Compound	X	*cis*-O-O	*trans*-O-O
Series *IX*			
86	3,5-Cl_2	1 755·0	1 739·0
87	2-NO_2	1 757·0	1 742·0
88	3-CF_3	1 754·0	1 738·0
89	3-CF_3, 4-Cl	1 756·0	1 740·0
90	3-Cl	1 754·0	1 738·0
91	4-Br	1 755·0	1 738·0
92	3,4-Cl_2	1 755·0	1 739·0
93	3-F	1 753·0	1 738·0
94	3-OCH_3	1 752·0	1 736·0
95	H	1 752·0	1 736·0
96	2-Cl	1 751·0	1 739·0
97	2-Br	1 751·0	1 738·0
98	2-OCH_3	1 741·0	1 729·0
Series *X*			
99	3-NO_2, 4-Cl	1 743·0	1 721·0
100	2-NO_2	1 741·0	1 722·0

Compound	X	*cis*-O-O	*trans*-O-O
Series *X*			
101	3,5-$(NO_2)_2$	1 742·0	1 721·0
102	3-CF_3, 4-Cl	1 743·0	1 726·0
103	3-NO_2	1 740·0	1 721·0
104	3,4-Cl_2	1 740·0	1 720·0
105	3-CF_3	1 740·0	1 720·0
106	3-Br	1 740·0	1 718·0
107	3-Cl	1 738·0	1 718·0
108	3-F	1 748·0	1 719·0
109	4-Br	1 739·0	1 717·0
110	2-Br	1 739·0	1 719·0
111	4-Cl	1 739·0	1 718·0
112	H	1 736·0	1 715·0
113	3-NH_2	1 737·0	1 715·0
114	4-CH_3	1 733·0	1 712·0
115	2-OCH_3	1 732·0	1 713·0
116	4-OCH_3	1 732·0	1 710·0
117	2-NH_2	1 730·0	1 711·0

TABLE II

Statistical Treatment of Linear Correlations between the Wavenumbers of the C=O Stretching Vibration and Substituent Constants

Series	Conf.	Eq.	n^a	r^b	s^c	ν^{0d}	ϱ^e	$s_\varrho{}^f$	r^{+g}	$s_{r+}{}^h$
I	*s-cis*	*1*	12	0·981	0·88	1 671·3	6·86	1·05	0·76	0·26
	s-cis	*2*	12	0·968	1·09	1 670·3	9·00	0·74	—	—
	s-cis	*3*	12	0·980	0·87	1 671·6	6·00	0·39	—	—
	s-trans	*1*	12	0·983	0·96	1 652·7	8·89	1·14	0·57	0·20
	s-trans	*2*	12	0·984	0·89	1 651·9	10·61	0·60	—	—
	s-trans	*3*	12	0·978	1·06	1 653·5	6·94	0·47	—	—
II	*s-cis*	*1*	10	0·977	1·13	1 672·6	7·28	1·56	0·60	0·32
	s-cis	*2*	10	0·972	1·19	1 671·8	8·67	0·75	—	—
	s-cis	*3*	10	0·976	1·10	1 673·2	5·64	0·45	—	—
	s-trans	*1*	10	0·992	0·85	1 652·4	9·92	1·17	0·47	0·16
	s-trans	*2*	10	0·986	1·05	1 651·9	10·90	0·66	—	—
	s-trans	*3*	10	0·995	0·63	1 653·6	7·12	0·26	—	—
III	*s-cis*	*1*	9	0·990	0·27	1 668·4	3·48	0·35	0·87	0·26
	s-cis	*2*	9	0·962	0·48	1 667·9	4·38	0·47	—	—
	s-cis	*3*	9	0·989	0·26	1 668·5	3·32	0·19	—	—
	s-trans	*1*	8	0·987	0·39	1 645·7	5·03	0·66	0·71	0·27
	s-trans	*2*	8	0·964	0·59	1 645·1	6·16	0·69	—	—
	s-trans	*3*	8	0·984	0·40	1 645·9	4·43	0·33	—	—
IV	*s-cis*	*1*	8	0·973	0·33	1 666·1	2·71	0·42	0·76	0·36
	s-cis	*2*	8	0·957	0·38	1 665·8	3·47	0·43	—	—
	s-cis	*3*	8	0·965	0·34	1 662·2	2·48	0·28	—	—
	s-trans	*1*	8	0·989	0·23	1 647·0	2·96	0·30	0·87	0·24
	s-trans	*2*	8	0·973	0·33	1 646·5	3·93	0·38	—	—
	s-trans	*3*	8	0·989	0·21	1 647·5	2·84	0·17	—	—
V	*s-cis*	*1*	13	0·969	1·05	1 659·3	4·11	1·58	1·73	0·95
	s-cis	*2*	13	0·927	1·51	1 658·3	8·38	1·02	—	—
	s-cis	*3*	13	0·968	0·56	1 658·8	4·20	0·35	—	—
VI	*s-cis*	*1*	12	0·961	1·42	1 660·6	5·03	1·59	1·71	0·85
	s-cis	*2*	12	0·905	2·07	1 658·5	9·84	1·46	—	—
	s-cis	*3*	12	0·954	1·46	1 659·0	6·82	0·68	—	—
	s-trans	*1*	12	0·952	0·87	1 641·5	2·39	0·97	2·12	1·26
	s-trans	*2*	12	0·886	1·25	1 640·0	5·35	0·89	—	—
	s-trans	*3*	12	0·939	0·92	1 640·9	3·73	9·43	—	—

TABLE II
(*Continued*)

Series	Conf.	Eq.	n^a	r^b	s^c	ν^{0d}	ϱ^e	$s_\varrho{}^f$	r^{+g}	$s_{r^+}{}^h$
VII	*s-cis*	*1*	11	0·974	0·69	1 662·8	4·12	0·84	0·73	0·35
	s-cis	*2*	11	0·959	0·78	1 662·0	5·19	0·51	—	—
	s-cis	*3*	11	0·973	0·63	1 663·0	3·42	0·27	—	—
	s-trans	*1*	13	0·987	0·67	1 639·8	8·04	0·72	0·30	0·12
	s-trans	*2*	13	0·986	0·65	1 639·6	8·15	0·42	—	—
	s-trans	*3*	13	0·963	1·04	1 641·0	5·28	0·45	—	—
VIII	*s-cis*	*1*	11	0·984	0·45	1 660·0	3·66	0·53	0·48	0·23
	s-cis	*2*	11	0·979	0·50	1 659·8	4·16	0·29	—	—
	s-cis	*3*	11	0·977	0·51	1 660·5	2·72	0·20	—	—
IX	*cis*-O—O	*1*	13	0·969	1·08	1 751·2	6·99	1·17	1·93	0·61
	cis-O—O	*2*	13	0·871	2·05	1 748·7	11·56	1·96	—	—
	cis-O—O	*3*	13	0·952	1·28	1 750·0	9·13	0·89	—	—
	trans-O—O	*1*	13	0·918	1·32	1 735·8	6·43	1·43	1·12	0·63
	trans-O—O	*2*	13	0·875	1·54	1 734·6	8·81	1·47	—	—
	trans-O—O	*3*	13	0·918	1·26	1 735·7	6·68	0·87	—	—
X	*cis*-O—O	*1*	19	0·956	1·21	1 736·8	6·93	0·91	0·73	0·29
	cis-O—O	*2*	19	0·934	1·42	1 735·9	8·37	0·76	—	—
	cis-O—O	*3*	19	0·953	1·20	1 737·2	6·21	0·48	—	—
	trans-O—O	*1*	19	0·926	1·66	1 715·4	8·61	1·25	0·30	0·26
	trans-O—O	*2*	19	0·910	1·76	1 715·3	8·74	0·96	—	—
	trans-O—O	*3*	19	0·903	0·83	1 716·7	6·30	0·73	—	—

[a] Number of experimental points used in correlation. [b] Correlation coefficient. [c] Standard deviation. [d] Intercept. [e] Slope. [f] Standard deviation of ϱ. [g] Yukawa–Tsuno coefficient. [h] Standard deviation of r^+.

Similarly to the case of aromatic carbonyl compounds[8] the series of aromatic α,β-unsaturated and arylfurancarbonyl compounds *I*–*X* exhibit statistically significant results when Yukawa–Tsuno equation is used in correlations between the C=O stretching fundamental and the substituent effects. The values of Yukawa–Tsuno coefficients r^+ for series of chalcones and their analogues were determined mostly in the region of 0·30–0·87 and indicate a significant portion of mesomeric effects in total substituent influence. The extremely high value of r^+ (1·71–2·39) in the case of series *V* and *VI* is caused by an electronowithdrawing effect of (4-nitrophenyl)-2-furyl and (4-chlorophenyl)-2-furyl groups, resp.

Treatment of infrared data from conformation isomers of chalcones, related series of substituted methyl styryl ketone and butyl styryl ketones by the Swain–Lupton[2,3] approach showed little difference in the values of the correlation coefficients or in the contribution of the resonance parameter (%R) to the correlations[3]. Thus analysis of the C=O stretching frequency by both the Yukawa–Tsuno and Swain–Lupton approach leads to the conclusion that differences, if any, between the transmission of resonance effects in the s-*cis* and s-*trans* conformers of α,β-unsaturated ketones are not detectable by these methods.

To investigate the transmission of substituent effects and the influence of conformation on substituent effects, it is convenient to use Yukawa-Tsuno equation in from of Eq. (*4*)

$$\nu = \nu^0 + \varrho^n\sigma^n + \varrho_{r^+}\,\Delta\sigma_{R^+}\,, \tag{4}$$

where ϱ^n is identical with ϱ in Eq. (*1*) and expresses the sensitivity of C=O group to the "normal" substituent effects (*i.e.*, to the inductive and field effects); $\varrho_{r^+} = r^+\varrho^n$ is a measure of sensitivity of carbonyl group to the resonance substituent effects. The values of ϱ_{r^+} obtained by correlations according to the Eq. (*4*) are listed in Table III. It is clear from the table that in series of chalcones and their analogues (*I* – *VIII*) the sensitivity of C=O group to the resonance effects is practically not affected by conformation. The series of compounds *VI* is, however, an exception since the C=O group is more sensitive to the resonance effects in *s-cis* as in *s-trans* conformation. It was already mentioned that in this series the portion of resonance effects in total substituent influence is extremely high. The C=O group of compounds *I* – *VIII* except the series *VI* is more sensitive to the "normal" substituent effects in *s-trans* conformation as in *s-cis* conformation. The cause is probably a field effect operating between the C=O and CH=CH groups[16,17] which might reduce the transmission ability of the whole system.

In series *IX* and *X* a high value of the coefficient r^+ can be observed, which is due to a strong resonance interaction between the substituents and C=O group. The resonance effects in both cases affect more efficiently the *cis*-O—O conformation than the *trans*-O—O conformation.

The application of Yukawa–Tsuno equation in the shape of Eq. (*4*) allows a separate investigation of the transmission of both resonance and "normal" substituent effects. Comparing the data obtained for the series *III*, *IV*, *IX*, and *X* with that of 1-phenyl-3-arylpropenones (*II*), substituted benzenecarboxylic acids (*XI*) (*cf.*[8]) and their methyl esters (*XII*) (*cf.*[9]) the transmissive factors of resonance effects (π'_M) and "normal" effects (π'_n) for the furan and thiophene rings can be calculated as follows:

$$\pi'_M(\mathrm{Fu}) = \varrho_{r^+}(III)/\varrho_{r^+}(II) = \varrho_{r^+}(IX)/\varrho_{r^+}(XI) = \varrho_{r^+}(X)/\varrho_{r^+}(XII) \tag{5a}$$

TABLE III

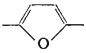
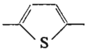
Statistical Values ϱ_r^+ for the Series *I*—*X*

Series	Conformation	ϱ_{r^+}	$s_{\varrho_{r^+}}$ [a]
I	*s-cis*	5·18	1·00
I	*s-trans*	5·07	1·09
II	*s-cis*	4·37	1·42
II	*s-trans*	4·68	1·07
III	*s-cis*	3·02	0·59
III	*s-trans*	3·55	0·89
IV	*s-cis*	2·07	0·65
IV	*s-trans*	2·58	0·46
V	*s-cis*	7·12	1·18
VI	*s-cis*	8·59	1·57
VI	*s-trans*	5·06	0·96
VII	*s-cis*	2·99	0·85
VII	*s-trans*	2·45	0·74
VIII	*s-cis*	1·77	0·54
IX	*cis*-O—O	13·47	1·99
IX	*trans*-O—O	7·19	2·43
X	*cis*-O—O	5·06	1·34
X	*trans*-O—O	2·56	1·84

[a] Standard deviation of ϱ_{r^+}.

TABLE IV

Transmissive factors of Resonance and "Normal" Substituent Effects for 2,5-Furylene and 2,5-Thienylene Bridging Groups

Bridging group	Series	Conformation	π'_M	π'_n
	*IX, XI*	*cis*-O—O	1·61 ± 0·41	0·59 ± 0·14
		trans-O—O	0·86 ± 0·38	0·54 ± 0·16
	X, XII	*cis*-O—O	0·51 ± 0·18	0·80 ± 0·20
		trans-O—O	0·26 ± 0·21	1·00 ± 0·22
	*III, II*	*s-cis*	0·69 ± 0·36	0·48 ± 0·15
		s-trans	0·70 ± 0·36	0·51 ± 0·13
	IV, II	*s-cis*	0·47 ± 0·30	0·30 ± 0·14
		s-trans	0·55 ± 0·22	0·57 ± 0·07

$$\pi'_n(\mathrm{Fu}) = \varrho_n(III)/\varrho_n(II) = \varrho_n(IX)/\varrho_n(XI) = \varrho_n(X)\varrho_n(XII) \tag{5b}$$

$$\pi'_M(\mathrm{Thi}) = \varrho_{r^+}(IV)/\varrho_{r^+}(II) \tag{5c}$$

$$\pi'_n(\mathrm{Thi}) = \varrho_n(IV)/\varrho_n(II)\,. \tag{5d}$$

The values of transmissive factors determined in this manner are given in Table IV. It is clear from the table that the value of transmissive factor of resonance effects for series of *cis*-O—O conformers of arylfurancarboxylic acids (*IX*) is anomalously high, *i.e.*, 1·61. Such a type of transmission when ($\pi' > 1$) can be regarded[18,19] as a positive bridge effect and may be accounted for an increase in coplanarity of C=O group and furan ring caused by an intramolecular hydrogen bonding between the OH and furylene group[12]. A relatively high value of π'_n observed in the case of methyl esters of arylfuranocarboxylic acids (*X*) points out the significant role of π-electrons in transmission of inductive effects. An extension of structure of *s-cis* and and *s-trans* conformers of 1-phenyl-3-arylpropenones by 2,5-furylene or 2,5-thienylene group (series *III* and *IV*) causes a decrease in the transmission of both the resonance and "normal" substituent effects approximately in the same measure. The comparison of transmissive factors in Table IV shows that 2,5-furylene group transmits the resonance as well as the "normal" effects more efficiently as 2,5-thienylene group. This is in a good accordance with the results of our previous investigations of transmission of polar substituent effects by furan and thiophene rings using Hammett and Brown correlations[5,20-24]. The efficiency of transmission of both the resonance and "normal" effects observed with series *III* and *IV* is always somewhat higher in the case of *s-trans* conformation than in *s-cis* conformation. As it was already mentioned[16], this effect can be explained by a better coplanarity of the double bonds in *s-trans* conformation compared with *s-cis* conformers.

Finally, it can be concluded that the application of Yukawa–Tsuno equation (in spite of larger statistical errors appearing by determination of correlation parameters[6,9]) provides some useful information about transmission of substituent effects by various systems in side-chains of substituted aromatic compounds.

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