

Application of the Seth-Paul—Van Duyse equation

VI. Calculation of substituent constants of complex structural fragments

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A general empirical formula for calculation of $X^+(R)$ substituent constants of complex structural fragments has been derived using substituent constants of single groups and Charton's and Jaffé's transmissive factors of fundamental structural units. The same formula is equally well usable in the case of calculation of Hammett σ and Brown—Okamoto σ^+ or σ^- constants of complex substituents. The Jaffé's transmissive factor γ for both the *s-cis* and *s-trans* conformations of an *E*-isomeric CH=CH group and some new $X^+(R)$ values of single substituents containing multiple bonds between carbon atoms have been determined. Transmissive factors γ and π' of several bridge groups were tabulated.

Выведена общая эмпирическая формула для расчета констант заместителей $X^+(R)$ сложных структурных фрагментов с помощью констант заместителей простых групп и трансмиссионных факторов основных структурных единиц по Чартону и Джаффе. Та же самая формула равным образом применима к расчету σ -констант сложных заместителей по Гаммету и σ^+ - или σ^- -констант по Браун—Окамото. Определен трансмиссионный γ -фактор Джаффе для *s-цис* и *s-транс* конформаций *E*-изомерной CH=CH группы и некоторые $X^+(R)$ величины простых заместителей, содержащих кратные СС связи. Трансмиссионные γ - и π' -факторы некоторых мостиковых групп сведены в таблицу.

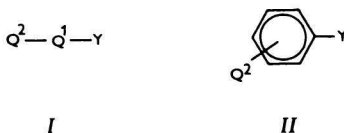
The previous papers [1—5] were devoted to the application of extended and improved Seth-Paul—Van Duyse equation [2]. In the case of cyclic 1,3-dicarbonyl compounds [1, 5] we tried to express the electronic effects of some more complex structural fragments using substituent constants and transmissive factors of single groups. The proposed equations were satisfactory for calculation of substituent constants of groups attached in the position 2 of cyclic 1,3-dicarbonyl systems, however in the case of monocarbonyl compounds they appeared to be invalid.

Recently, several physical properties concerning the C=O group have been published for a great number of organic structures. Especially, infrared carbonyl stretching frequencies of many organic compounds were measured under nearly standard conditions, *i.e.* in dilute solutions of CCl₄. Most of these compounds contained complex substituents or structural fragments attached to the C=O group.

In order to examine the applicability of the improved Seth-Paul—Van Duyse equation to the C=O stretching frequencies of further organic compounds, the main goal of the present work was to derive an empirical equation for calculation of substituent constants of complex structural fragments and determine or collect several transmissive factors and substituent constants necessary for the above calculations.

Results and discussion

Charton [6] compared the reaction constants (ρ) of Hammett type correlations of compounds *I* with those of substituted benzene derivatives *II*



where Y is a reaction (or other electron-active) site and defined the transmissive factor $\gamma(Q^1)$ of structural group Q^1

$$\gamma(Q^1) = \rho(I)/\rho(II) \quad (1)$$

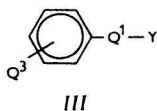
The value of $\gamma(Q^1)$ expresses the relative change of electronic effect of substituent Q^2 connected to the Q^1 group in comparison with the effect of the same substituent attached to the benzene ring.

According to this consideration the substituent constant $C(Q^2-Q^1)$ of the substituted Q^1 group can be expressed by the subsequent equation

$$C(Q^2-Q^1) = C'(Q^1) + \gamma(Q^1)C(Q^2) \quad (2)$$

where $C'(Q^1)$ stands for the substituent constant of Q^1 group attached directly to the electron-active site and $C(Q^2)$ is the substituent constant of Q^2 group attached to the benzene ring.

The prolongation of the substituent group by a further structural unit Q^3 requires the introduction of Jaffé's transmissive factors $\pi'(Q^1)$ [7]. Comparing the reaction constants of structure—reactivity correlations for the series *III*



with those of *II* the transmissive factors $\pi'(Q^1)$ can be expressed as follows

$$\pi'(Q^1) = \rho(III)/\rho(II) \quad (3)$$

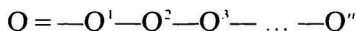
The value of $\pi'(Q^1)$ characterizes the relative change of electronic effect of the substituted benzene ring by insertion of a structural unit Q^1 between the electron-active site Y and this ring.

Applying the above definitions of both transmissive factors $\gamma(Q)$ and $\pi'(Q)$ the substituent constant $C(Q^3-Q^2-Q^1)$ of a more complex structural fragment $Q^3-Q^2-Q^1-$ can be given by the equation

$$C(Q^3-Q^2-Q^1) = C'(Q^1) + \gamma(Q^1)C(Q^2) + \pi'(Q^1)\gamma(Q^2)C(Q^3) \quad (4)$$

where $C(Q^3)$ stands for the substituent constant of group Q^3 attached to the benzene ring and the remaining constants have an analogical meaning as in eqn (2).

A further prolongation of the complex substituent group requires the extension of eqn (4) by additional terms creating a sequence. According to this the substituent constant $C(Q)$ of a complex structural fragment Q containing n of Q^i structural units



can be expressed by a general formula

$$C(Q) = C'(Q^1) + \gamma(Q^1)C(Q^2) + \sum_{i=3}^n \gamma(Q^{i-1})C(Q^i) \prod_{j=1}^{i-2} \pi'(Q^j) \quad (5)$$

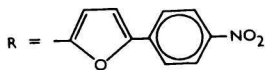
Employing eqn (5) to the calculation of $X^+(R)$ values of structural fragments in conception of the improved Seth-Paul—Van Duyse equation [2]

$$C'(Q^1) = X^+(Q^1)$$

and

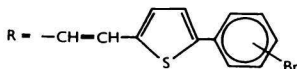
$$C(Q^2) = \delta^+(Q^2), \quad C(Q^3) = \delta^+(Q^3), \dots \quad C(Q^n) = \delta^+(Q^n)$$

The following two examples demonstrate the application of eqn (5) to the calculation of $X^+(R)$ constants of complex structural fragments R , e.g. for



$$X'(R) = X'(2-Fu) + \gamma(2-Fu)\delta'(4-Ph) + \pi'(2,5-Fu)\gamma(Ph)\delta'(4-NO_2)$$

and for



$$X'(R) = X'(CH=CH_2) + \gamma(CH=CH)\delta'(4-(2-Thi)) + \\ + \pi'(CH=CH)\gamma(2-Thi)\delta'(4-Ph) + \pi'(CH=CH)\pi'(2,5-Thi)\gamma(Ph)\delta'(3-Br)$$

The validity of the above derived eqn (5) in the calculation of $X'(R)$ constants of a great number of complex structural fragments containing conjugated multiple bonds, aromatic and heteroaromatic rings has been proved and the calculated $\Sigma X'(R)$ values were correlated with carbonyl stretching frequencies [8, 9].

Eqn (5) can be employed successfully also to the calculation of $\sigma_{..}$, σ or $\sigma_{..}^+$, $\sigma_{..}$, σ^+ and σ^- constants of complex substituents for Hammett and Brown equations, respectively. In the case of $\sigma_{..}$, $\sigma_{..}^+$ or $\sigma_{..}^-$ constants in eqn (5)

$$C'(Q^1) = \sigma_{..}(Q^1), \quad \sigma_{..}^+(Q^1) \text{ resp. } \sigma_{..}^-(Q^1)$$

$$C(Q^1) = \sigma(Q^1), \quad \sigma^+(Q^1) \text{ resp. } \sigma^-(Q^1)$$

for *para* or *meta* position of a Q^1 group attached to the benzene ring. By the calculation of σ , σ^+ or σ^- values

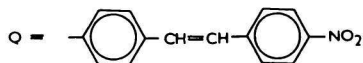
$$C'(Q^1) \equiv \sigma_{..}(Ph) = 0$$

$$\gamma(Q^1) \equiv \gamma(Ph) = 1$$

and eqn (5) acquires (e.g. for Hammett σ constants) a more simple shape

$$\sigma(Q) = \sigma(Q^2) + \sum_{i=1}^n \gamma(Q^{i-1})\sigma(Q^i) \prod_{j=1}^{i-1} \pi'(Q^j) \quad (6)$$

For example, according to eqn (6) the Hammett σ constant of a complex substituent



in the position 4 on the benzene ring can be given as follows

$$\sigma(4-Q) = \sigma(4-Ph) + \pi'(Ph)\sigma(4-CH=CH_2) + \\ + \pi'^2(Ph)\gamma(CH=CH)\sigma(4-Ph) + \pi'^2(Ph)\pi'(CH=CH)\sigma(4-NO_2)$$

Table 1

Comparison of calculated Hammett σ and Brown σ^+ constants of some complex substituents Q with experimental σ and σ^+ values

Q''	Position	Calculated ^b	Experimental ^c
Hammett σ constants			
4-NO ₂ Ph	4	0.19	0.23
3-NO ₂ Ph	4	0.16	0.17
3-ClPh	4	0.09	0.09
3-BrPh	4	0.09	0.08
4-ClPh	4	0.05	0.05
4-MePh	4	-0.05	-0.05
4-OMePh	4	-0.08	-0.09
4-NH ₂ Ph	4	-0.18	-0.21
3-BrPh	3	0.09	0.08
<i>E</i> -PhCH=CH	4	-0.03 ^d	-0.05
<i>E</i> -NO ₂ CH=CH	4	0.38 ^d	0.26
<i>E</i> -CHOCH=CH	4	0.19 ^d	0.13
<i>E</i> -CO ₂ HCH=CH	4	0.27 ^d	0.23
<i>E</i> -PhCOCH=CH	3	0.26 ^d	0.18
<i>E</i> -MeCOCH=CH	4	0.07 ^d	-0.01
PhC≡C	4	0.22	0.19 ^e
MeC≡C	4	0.18	0.09
CF ₃ C≡C	4	0.50	0.51
CF ₃ C≡C	3	0.48	0.41
PhCO	4	0.41	0.40
5-NO ₂ (2-Fu)	4	0.29	0.20
5-Br(2-Fu)	4	0.09	0.00
5-Me(2-Fu)	4	-0.05	-0.17
5-Br(2-Fu)	3	0.17	0.15
Brown σ^+ constants			
4-NO ₂ Ph	4	0.03	0.03
3-ClPh	4	-0.08	-0.15
4-BrPh	4	-0.14	-0.18
4-NO ₂ Ph	3	0.21	0.18
MeCO	4	0.46	0.52 ^d
PhCO	4	0.57	0.51

a) Abbreviations: Ph — phenyl, Me — methyl, Fu — furyl, *E* — *E*-isomers regarding the plane of C=C bond.

b) σ Constants calculated according to eqn (6).

c) Determined from kinetic data and taken from [10].

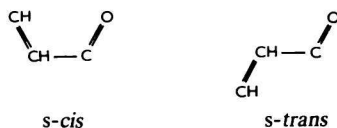
d) Calculated for *s-trans* conformation of C=C bond in respect to the reaction site.

e) Taken from [11].

f) Taken from [12].

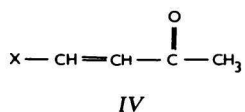
In Table 1 are listed some σ and σ^+ constants of complex substituents Q calculated by eqn (6) and compared with those determined experimentally from reaction kinetic data. The calculated values are in a very good agreement with the experimental ones, which is a good criterion of the applicability of the above-described approach to the Hammett and Brown equations.

In a number of complex substituents the $\text{CH}=\text{CH}$ group exists as a structural unit. If this group is attached directly to the $\text{C}=\text{O}$ group, which is the electron-active site of the molecule, the occurrence of two nearly planar conformations *s-cis* and *s-trans* (Scheme 1) can be expected.



Scheme 1

As the transmissive factors $\gamma(\text{CH}=\text{CH})$ for *s-cis* and *s-trans* conformations of a vinylenic group have not been published yet, we determined them using available carbonyl stretching frequencies of *E*-isomers of substituted propenones *IV* (measured in dilute solutions of CCl_4).



The data and σ_p^+ substituent constants of groups X are given in Table 2. Correlating the $\nu(\text{C}=\text{O})$ values of series *IV* with σ_p^+ constants the following results were obtained

$$\nu(\text{C}=\text{O})_{s\text{-trans}} = 22.738\sigma_p^+(\text{X}) + 1681.7 \quad (7)$$

$$r = 0.954, \quad s = \pm 1.7 \text{ cm}^{-1}$$

$$\nu(\text{C}=\text{O})_{s\text{-cis}} = 27.305\sigma_p^+(\text{X}) + 1703.9 \quad (8)$$

$$r = 0.974, \quad s = \pm 1.6 \text{ cm}^{-1}$$

r and s are the correlation coefficient and standard deviation, respectively.

From the comparison of the slopes of above linear relationships (eqns (7) and (8)) with that of an analogical correlation (eqn (9)) for 66 derivatives of acetophenone (*V*) [17]

$$\nu(\text{C}=\text{O}) = 11.467\sigma^+(\text{X}) + 1691.3 \quad (9)$$

$$r = 0.992, \quad s = \pm 0.2 \text{ cm}^{-1}$$

Table 2

Carbonyl stretching frequencies measured in CCl_4 and σ_p^+ substituent constants of *E*-isomers of substituted propenones IV

X ^a	$\nu(\text{C}=\text{O})/\text{cm}^{-1}$		Ref.	$\sigma_p^+(\text{X})^b$
	<i>s-trans</i>	<i>s-cis</i>		
H	1684	1706	[13]	0
Me	1676	1697	[13]	-0.31
Ph	1676.4	1697.7	[14]	-0.18
Fc	1665	1684	[15]	-0.71
2-Thi	1674.7	1695.3	[16]	-0.38
Me ₂	—	1686	[13]	-0.62 ^c
4-PhPh	1674	1696.9	[13, 14]	-0.24
4-ClPh	1677.2	1699.2	[14]	-0.19
4-BrPh	1678.3	1699.3	[14]	-0.18
4-NO ₂ Ph	1680.8	1702	[14]	0.03

a) Abbreviations: Fc — ferrocenyl, Thi — thienyl.

b) Taken from [2, 10].

c) Calculated as $2\sigma_p^+(\text{Me})$.

we can determine the transmissive factors γ for both the *s-trans* and *s-cis* conformations of the $\text{CH}=\text{CH}$ group as follows

$$\gamma(\text{CH}=\text{CH})_{s\text{-trans}} = \rho(\text{IV})_{s\text{-trans}}/\rho(\text{V}) = 1.988$$

$$\gamma(\text{CH}=\text{CH})_{s\text{-cis}} = \rho(\text{IV})_{s\text{-cis}}/\rho(\text{V}) = 2.381$$

The value of $\gamma(\text{CH}=\text{CH})_{s\text{-cis}}$ is in a reasonable good agreement with that determined previously by Charton [6] ($\gamma(\text{CH}=\text{CH}) = 2.23$) using correlations between ionization constants of carboxylic acids and substituent constants. The transmissive factors $\gamma(\text{Q})$ and $\pi'(\text{Q})$ of some fundamental structural units Q recommended in the application of eqn (5) are collected in Table 3.

In order to calculate the $X^+(\text{R})$ values of complex substituents, it was also necessary to determine the $X^+(\text{R})$ constants of some further structural fragments lacking in the present literature.

In the case of aromatic or heteroaromatic groups R attached directly to a carbonyl group and possessing an electron-donating effect eqn (10) derived previously [2] can be used.

$$X^+(\text{R}) = 0.238\sigma^+(\text{R}) + 1.077 \quad (10)$$

However, this equation for nonaromatic groups in the role of substituents appeared to be invalid.

Table 3

Transmissive factors $\gamma(Q)$ and $\pi'(Q)$ of some fundamental structural units

Q	$\gamma(Q)$	Ref.	$\pi'(Q)$	Ref.
Benzene	1	<i>a</i>	0.26	[18]
1,4-Naphthalene	1	[5]	0.26	[5]
1,1'-Ferrocene	0.93	[5]	0.25	[19]
1,3-Ferrocene	1.41	[5]	0.38	[19]
2,5-Furan	1.40	[20, 21]	0.80 ^b , 0.98 ^c	[4]
2,5-Thiophene	1.09	[20, 21]	0.44	[22]
<i>E-s-trans</i> -CH=CH	1.99	<i>d</i>	0.85	[3]
<i>E-s-cis</i> -CH=CH	2.38	<i>d</i>	0.77	[3]
C≡C	1.89	[6]	0.33	[18]
C=O	3.34	[23]	0.43	[18]
<i>trans</i> -1,2,-Cyclopropane	1.97	[23]	0.37	[18, 24, 25]
1,1-Cyclopropane	5.36	[23]	—	—
C=CH ₂	4.25	[23]	—	—
C=NOH	2.37	[23]	—	—
2,5-Selenophene	1.23	[21]	—	—
2,5-Pyrrole	1.65	[21]	—	—
2,5-Tellurophene	1.20	[21]	—	—
3,5-Pyridine	0.95	[26, 27]	—	—
2,5-Pyridine	1.04	<i>e</i>	—	—
2,5-Thiazole	1.10	<i>e</i>	—	—
2,6-Benzothiazole	0.35	[47]	—	—
2,9-Fluorene	0.69	[29]	—	—

a) From definition of $\gamma(Q)$ by eqn (1).

b) For O—O—*trans* conformation.

c) For O—O—*cis* conformation.

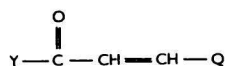
d) This paper.

e) Calculated using the results of paper [28].

Therefore, we employed for the determination of $X^+(R)$ constants of structural fragments CH=CH₂ and C≡CH eqn (6) and the improved Seth-Paul—Van Duyse equation (eqn (11)) [2]

$$\nu(C=O) = 38.219 \Sigma X^+(R) + 1583.426 \quad (11)$$

Thus, the $X^+(CH=CH_2)$ constants for *s-trans* and *s-cis* conformations can be determined according to the following expression (eqn (12)) using $\Sigma X^+(R)$ values calculated from eqn (11) for fundamental structural types of compounds VI.



VI

$$X'(\text{CH}=\text{CH}_2) = \Sigma X^+(\text{R}) - X^+(\text{Y}) - \gamma(\text{CH}=\text{CH})\delta^+(4-\text{Q}) \quad (12)$$

The $X'(\text{R})$ constants of a vinylenic group can be given by arithmetic means of values listed in Table 4

$$X^+(\text{CH}=\text{CH}_2)_{s\text{-trans}} = 0.785$$

$$X^+(\text{CH}=\text{CH}_2)_{s\text{-cis}} = 1.338$$

Table 4

Determination of $X'(\text{CH}=\text{CH}_2)$ constants according to eqns (11) and (12)^a

Y ^b	Q ^b	$\nu(\text{C}=\text{O}) (\text{CCl}_4)/\text{cm}^{-1}$				$X'(\text{CH}=\text{CH}_2)$	
		<i>s-trans</i>	Ref.	<i>s-cis</i>	Ref.	<i>s-trans</i>	<i>s-cis</i>
Me	H •	1684	[13]	1706	[13]	0.825	1.400
Me	Me	1676	[13]	1697	[13]	0.682	1.325
Ph	Ph	1653	[30]	1672	[30]	0.822	1.334
Me	Ph	1676.4	[14]	1697.7	[14]	0.698	1.269
Bu	Ph	1675	[31]	1695	[31]	0.718	1.255
Et	Ph	1674.6	[32]	1697.2	[32]	0.700	1.305
i-Pr	Ph	1671	[13]	1694	[13]	0.655	1.271
Me	Et	1682	[13]	1701	[13]	0.899	1.421
Me	Pr	1681	[13]	1702	[13]	0.865	1.438
Me	i-Pr	1683	[13]	1702	[13]	0.917	1.438
Pr	Ph	1672.5	[32]	1695.4	[32]	0.652	1.265
Pe	Ph	1673	[32]	1694	[32]	0.666	1.229
i-Bu	Ph	1669.3	[32]	1693.7	[32]	0.575	1.227
<i>t</i> -Bu	H	1684	[13]	1696	[13]	0.974	1.287
i-Pr	H	1682	[13]	1702	[13]	0.871	1.394
Pr	H	1686	[13]	1705	[13]	0.933	1.430
Me	2-Thi	1674.7	[16]	1695.3 ^b	[16]	0.746	1.318
Me	Fc	1665	[15]	1684	[15]	0.649	1.211
Ph	H	1661	[13]	1677	[13]	0.960	1.378
Et	H	1690	[13]	1707	[13]	1.004	1.475
Ph	Fc	1640	[33]	1665.5	[33]	0.500	1.463
Ph	2-Fu	1643	[17]	1669	[34]	0.688	1.407
Ph	2-Thi	1641	[17]	1663	[35]	0.601	1.210
H	Ph	1689	[13]	—	—	0.711	—
H	H	1704	[13]	—	—	0.999	—
H	2-Thi	1688	[16]	—	—	0.771	—

Table 4 (Continued)

Y ^b	Q ^b	$\nu(\text{C}=\text{O}) (\text{CCl}_4)/\text{cm}^{-1}$				$X^+(\text{CH}=\text{CH}_2)$	
		s-trans	Ref.	s-cis	Ref.	s-trans	s-cis
H	2-Fu	1688	[36]	—	—	0.805	—
H	Me	1699	[13]	—	—	1.027	—
NMe ₂	Ph	—	—	1658.1	[37]	—	1.478
OEt	Ph	—	—	1717	[38]	—	1.011
<i>t</i> -Bu	Ph	—	—	1688.7	[39]	—	1.182
<i>t</i> -Bu	2-Thi	—	—	1684.5	[16]	—	1.185
<i>t</i> -Bu	2-Fu	—	—	1684	[36]	—	1.212
2-Thi	Ph	—	—	1656	[39]	—	1.303
2-Thi	2-Thi	—	—	1648	[34]	—	1.206
Fc	Ph	—	—	1660	[33]	—	1.334
2-Fu	Ph	—	—	1667	[34]	—	1.420
Fc	Fc	—	—	1658	[3]	—	1.581
2-Fu	Fc	—	—	1661.5	[17]	—	1.463
2-Thi	Fc	—	—	1656	[17]	—	1.603
2-Fu	2-Fu	—	—	1667	[34]	—	1.572
OH	Ph	—	—	1733	[40]	—	0.900
OMe	Ph	—	—	1727	[41]	—	1.073
NMe ₂	Me	—	—	1665	[42]	—	1.732
2-Sel	Ph	—	—	1661	[43]	—	1.344
Mean values:						0.785	1.338

a) The $X^+(\text{Y})$ and $\delta^+(4\text{-Q})$ values were taken from [2, 3] except for $X^+(2\text{-Sel}) = 0.772$ and $X^+(\text{Fc}) = 0.756$, which have been determined by eqn (10) using $\sigma_{\text{r}}^+(2\text{-Sel}) = -1.28$ [44] and $\sigma_{\text{r}}^+(\text{Fc}) = -1.35$ [45], respectively.

b) Abbreviations: Bu — butyl, Et — ethyl, *i*-Pr — isopropyl, Pr — propyl, Pe — pentyl, *i*-Bu — isobutyl, *t*-Bu — *tert*-butyl, Sel — selenienyl.

In a similar manner we determined the $X^+(\text{R})$ constant of the $\text{C}\equiv\text{CH}$ structural fragment using carbonyl stretching frequencies of a series of phenylbenzoylacetylenes [46]

$$X^+(\text{C}\equiv\text{CH}) = 0.726$$

The applicability of above reported new $X^+(\text{R})$ constants has been proved in correlations between the carbonyl stretching frequencies and $\Sigma X^+(\text{R})$ values of a number of compounds containing multiple bonds between carbon atoms [8, 9].

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