

# Correlation relationships of molar refraction and ten topological indices for 47 organotin compounds<sup>\*</sup>

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**Abstract** Correlation relationships of 10 topological indices and molar refraction for 47 structurally-complicated organotins which included 16 ionic compounds  $R_mSnX_{4-m}$  and 31 covalent ones  $R_4Sn$  that is 41 aliphatic compounds (15 unsaturated and 26 saturated) and 6 aromatic ones were studied. Suitability of these ten topological parameters for describing the structure of elemental organic compounds was then evaluated according to the correlation results. Two lately improved molecular connectivity indices (*MCI*s)-radius-corrected  $MCI^{1X}$  and bond-length-corrected  $MCI^{1X^b}$  were applied and proved to be most suitable for the structure expression in QSA(P)R studies of organotins or other elemental organic compounds.

**Keywords:** QSA(P)R; organotin compounds; topological parameters; bond-length-corrected *MCI*; radius-corrected *MCI*.

## 1 Introduction

Quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies which provide tools to predict biological activities or environmental physicochemical properties of a compound based on molecular structure have become well established for organic pollutants. However, for elemental organic compounds, QSA(P)R studies have just been noted.

Selecting suitable structural parameters and correct function patterns is critical for the accuracy of QSA(P)R studies. Since elemental organic compounds have their own structural features, such as containing more non-carbon atoms (heteroatoms), the suitability of those descriptors which have been successfully applied in QSA(P)R studies for organic compounds is necessary to be reexamined.

Graph theory is largely applied to the characterization of chemical structures, as well as to the correlation studies of structure-property and structure-activity relationships, by means of so-called topological indices. These are numerical quantities based on various invariant or

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characteristics of a molecular graph. Due to their high predicting ability for different types of biological activities or other physicochemical properties (Sabljic, 1984; Richard, 1988), as well as their non-experiment and simplicity in calculation, many topological indices have been widely used in QSA(P)R studies.

The molar refraction (MR) has been referred as steric parameter in many QSAR references (Hansch, 1979). Hence, it has been applied in the correlation of  $\delta$  value of heteroatoms in attempt to obtain more accurate molecular connectivity indices. This paper studied the correlation relationships of MR and eight steric topological parameters ( ${}^1X$ ,  ${}^1X^v$ ,  $W$ ,  $I_D^w$ ,  $\bar{I}_D^w$ ,  $IC$ ,  $SIC$  and  $CIC$ ), which have been often used in many kinds of QSA(P)R studies for organic compounds, for 47 structurally-complicated organotin compounds which included 16 ionic compounds  $R_mSnS_{4-m}$ , 31 covalent ones  $R_4Sn$  that is 41 aliphatic compounds (15 unsaturated and 26 saturated), 6 aromatic ones. Two lately-improved  $MCI$ s-radius-corrected  $MCI {}^1X^r$  and bond-length-corrected  $MCI {}^1X^b$  were used, and their advantages for structure expression of elemental organic compounds were also evaluated.

## 2 Mechanism and calculation methods

The ten topological parameters used in this paper belong in three catalogs: (1) Molecular connectivity indices; (2) Wiener information indices; (3) Information content indices. Mechanism and calculation methods of each index are described briefly as follows:

### 2.1 Molecular connectivity indices ( $MCI$ s)

First order  $MCI {}^1X$ ; first order covalence  $MCI {}^1X^v$ , radius-corrected  $MCI {}^1X^r$  and bond-length-corrected  $MCI {}^1X^b$  (Kier, 1983) were used.

$MCI$ s are based on hydrogen-suppressed graph. First order  $MCI {}^1X$  can be calculated according to the following equation:

$${}^1X = \sum (\delta_i \delta_j)^{-1/2}, \quad (1)$$

where  $\delta$  value is the number of nonhydrogen atoms bonded to the atom in the molecule. However  ${}^1X$  can not distinguish unsaturation or heteroatoms. For example,  $(C_4H_9)_2(CH_2=CH)SnBr$  and  $(C_4H_9)_2(C_2H_5)SnI$  have the same  ${}^1X$  value of 2.561. To amend this limitation, Kier and Hall (Kier, 1981) have suggested the concept of valence  $MCI$  based on valence delta values,  $\delta^v$ , which is obtained from the following equation:

$$\delta^v = (Z^v - h)/(Z - Z^v - 1), \quad (2)$$

where  $Z^v$  is the number of valence electrons,  $h$  is the number of attached hydrogen atoms, and  $Z$  is the total number of electrons of the atom.  ${}^1X^v$  is calculated as follows:

$${}^1X^v = \sum (\delta_i^v \delta_j^v)^{-1/2}. \quad (3)$$

The valence  $MCI$  has been proved to be suitable for unsaturation and heteroatoms such as N, O, Cl, Br and I. However its suitability for elemental organic compounds is still to be verified.

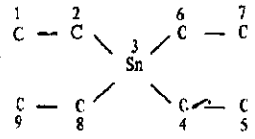
Radius-corrected  $MCI {}^1X^r$  and bond-length-corrected  $MCI {}^1X^b$  for 47 organotins were al-

so calculated as described in the following section.

## 2.2 Wiener information indices

Wiener number  $W$ , information index  $\bar{I}_D^w$  and mean information index  $\bar{I}_D^w$  (Bonchev, 1977) were calculated.

Wiener information indices are based on hydrogen-suppressed graph. Main calculation steps are explained briefly with the example of tetraethyltin. Fig. 1



The hydrogen-suppressed graph of tetraethyltin

(1) Write out the hydrogen-suppressed graph  $G$  of the molecule, and assign numbers to each atom (Fig. 1).

(2) Give  $N \times N$  distance matrix  $D(G)$  of the graph  $G$  with the entry  $d_{ij}$ .

$$D(G) = \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 3 & 1 & 3 & 4 \\ 1 & 0 & 1 & 2 & 3 & 2 & 3 & 2 & 3 \\ 2 & 1 & 0 & 1 & 2 & 1 & 2 & 1 & 2 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 3 \\ 4 & 3 & 2 & 1 & 0 & 3 & 4 & 3 & 4 \\ 3 & 2 & 1 & 2 & 3 & 0 & 1 & 2 & 3 \\ 4 & 3 & 2 & 3 & 4 & 1 & 0 & 3 & 4 \\ 3 & 2 & 1 & 2 & 3 & 2 & 3 & 0 & 1 \\ 4 & 3 & 2 & 3 & 4 & 3 & 4 & 1 & 0 \end{bmatrix}$$

where  $N$  is the number of atoms in graph  $G$ ,  $d_{ij}$  is defined as the number of bonds between atom  $i$  and atom  $j$  by the shortest path,  $N(G)$  is a symmetric matrix for  $d_{ij}=d_{ji}$ .

(3)  $W$ ,  $I_D^w$  and  $\bar{I}_D^w$  are defined as follows:

$$W = \sum_{ij} d_{ij}/2, \quad (4)$$

$$I_D^w = W \log_2 W - \sum K_d d \log_2 d, \quad (5)$$

$$\bar{I}_D^w = I_D^w/W, \quad (6)$$

where  $K_d$  is the times that the value  $d$  appears in the  $G$  partition. The  $W$ ,  $I_D^w$  and  $\bar{I}_D^w$  values for tetraethyltin were calculated according to the above equations:

$$W=88,$$

$$I_D^w = 88 \log_2 88 - 10 \times 2 \log_2 2 - 12 \times 3 \log_2 3 - 6 \times 4 \log_2 4 = 443.371,$$

$$\bar{I}_D^w = 443.371/88 = 5.038.$$

## 2.3 Information content indices

Information content  $IC$ ; structural information content  $SIC$  and complementary information content  $CIC$  (Sarkar, 1948) were calculated.

The total (nonhydrogen-suppressed) molecular graph is adopted to define the various indices of information content series. Calculation steps are as follows with the example of dimethyl (ethenyl) tin chloride.

(1) Write out the nonhydrogen-suppressed graph of the molecule, then assign a coordinate to each atom  $i$  in a pattern of  $e_{ij}^{v_i}$  (Fig. 2).  $e_{ij}$  is the number of bond between atom  $i$  and

atom  $j$ , and  $V_{ij}$  is the number of valence electrons of atom  $j$ .

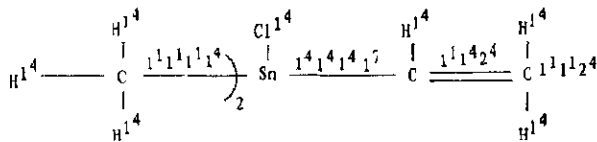


Fig. 2 Coordinate-attached structure of  $(\text{CH}_3)_2(\text{CH}_2=\text{CH})\text{SnCl}$

(2) Divide atoms of the molecule into disjoint partitioned subsets  $t$  such that atoms with the same  $e_{ij}^{v_j}$  lie in the same subset.  $n_t$  is defined as the number of atoms in the subset  $t$ .  $n$  is the total number of atoms in the molecule.

(3)  $IC$ ,  $SIC$  and  $CIC$  are then calculated as follows:

$$IC = - \sum_{i=1}^t (n_i/n) \log_2(n/nt), \quad (7)$$

$$SIC = IC/\log_2 n, \quad (8)$$

$$CIC = \sum_{i=1}^t (n_i/n) \log_2 n_i. \quad (9)$$

Consequently, calculation of  $IC$ ,  $SIC$  and  $CIC$  of  $(\text{CH}_3)_2(\text{CH}_2=\text{CH})\text{SnCl}$  based on Fig. 2 was given as follows:

$$IC = (9/15) \log_2(15/9) + (2/21) \log_2(21/2) + (4 \times 1/21) \log_2(21/1) = 1.602$$

$$SIC = 1.602/\log_2 15 = 0.410$$

$$CIC = (9/15) \log_2 9 + (2/21) \log_2 2 + (4 \times 1/21) \log_2 1 = 1.997$$

MR values for the 47 organotins studied in this paper were calculated using Lorentz-Lorenz equation:

$$\text{MR} = [(n^2 - 1)/(n^2 + 2)](M/d), \quad (10)$$

where  $M$  is the molecular weight,  $n$  is the index of refraction and  $d$  is the density.  $n_D^{20}$  and  $d_4^{20}$  values for the 47 organotins were obtained from the literature compilations of Weast (Weast, 1977).

### 3 Results and discussion

Valence  $\delta$  values of heteroatoms studied in this paper were calculated according to Equation (2) and listed in Table 1.

Table 1  $\delta^v$  values of atoms

Atom	$\delta^v$	Atom	$\delta^v$	Atom	$\delta^v$
—Sn—	0.089	—C—	4.000	—Sn—	6.000
—CH—	3.000	—Cl	0.778	—CH <sub>2</sub> —	2.000
—Br	0.259	—CH <sub>3</sub>	1.000	—I	0.156
—CH=	3.000				

The values of  ${}^1X$ ,  ${}^1X^v$ ,  $\ln W$ ,  $\ln I_D^w$ ,  $\bar{I}_D^w$ ,  $IC$ ,  $SIC$ ,  $CIC$  and  $MR$  for 47 organotins are listed in Table 2. Correlation coefficients of  $MR$  and these topological indices are listed in Table 3.

Table 2 Topological indices and MR values for 47 organotins

Compounds	$MR$	${}^1X$	${}^1X^v$	${}^1X^r$	${}^1X^b$	$\ln W$	$\ln I_D^w$	$\bar{I}_D^w$	$IC$	$SIC$	$CIC$
1 $(CH_3)_4Sn$	35.769	2.000	13.416	2.697	2.818	2.773	3.951	3.250	1.086	0.266	3.001
2 $(C_2H_5)_4Sn$	58.481	4.243	12.515	4.735	4.821	4.477	6.094	5.038	1.326	0.273	3.532
3 $(C_3H_7)_4Sn$	73.995	6.243	14.315	6.735	6.821	5.545	7.357	6.123	1.294	0.242	4.064
4 $(C_4H_9)_4Sn$	92.119	8.243	16.315	8.735	8.821	6.328	8.260	6.907	1.254	0.219	4.474
5 $(i-C_4H_9)_4Sn$	92.598	7.926	14.517	8.328	8.398	6.223	8.159	6.934	1.462	0.255	4.266
6 $(C_5H_{11})_4Sn$	110.642	10.243	18.315	10.735	10.821	6.947	8.965	7.521	1.219	0.202	4.803
7 $(i-C_5H_{11})_4Sn$	111.359	9.926	16.517	10.338	10.398	6.875	8.895	7.538	1.465	0.243	4.557
8 $(C_8H_{17})_4Sn$	165.760	16.243	24.315	16.735	16.821	8.278	10.456	8.829	1.148	0.172	5.510
9 $(C_{12}H_{25})_4Sn$	249.776	24.243	32.315	24.735	24.821	9.448	11.748	9.971	1.094	0.152	6.125
10 $(CH_3)_3(C_{10}H_{21})Sn$	79.705	6.561	17.141	7.206	7.319	6.050	7.878	6.223	1.284	0.235	4.176
11 $((CH_3)_3(C_{12}H_{25}))Sn$	88.877	7.561	18.141	8.206	8.319	6.466	8.354	6.608	1.263	0.224	4.381
12 $(CH_2=CH)_4Sn$	52.309	4.243	9.379	3.190	4.472	4.477	6.094	5.038	1.582	0.360	2.811
13 $(CH_2=CH-CH_2)_4Sn$	70.590	6.243	12.753	5.173	6.472	5.545	7.357	6.123	1.698	0.337	3.347
14 $(CH_2=CH)Sn(CH_3)_3$	40.823	2.561	12.407	2.820	3.232	3.332	4.667	3.798	1.516	0.364	0.654
15 $(CH_2=CH-CH_2)Sn(CH_3)_3$	45.838	3.061	13.251	3.316	3.732	3.829	5.273	4.241	1.628	0.371	2.765
16 $(CH_2=CH)_2Sn(C_4H_9)_2$	72.007	6.243	12.847	5.963	6.647	5.591	7.401	6.110	1.654	0.318	3.555
17 $(CH_2=CH)_3Sn-C_{10}H_{21}$	91.123	8.243	14.113	7.576	8.560	6.534	8.452	6.810	1.613	0.290	3.941
18 $(CH_2=CH)_3Sn-C_6H_{13}$	72.515	6.243	12.113	5.576	5.560	5.649	7.452	6.067	1.723	0.336	3.407
19 $(CH_2=CH)_3SnC_8H_{17}$	82.127	7.243	13.113	6.576	7.560	6.123	7.988	6.462	1.666	0.311	3.692
20 $C_4H_9SnCl_3$	50.818	3.561	15.488	3.051	4.533	4.263	5.793	4.620	1.850	0.453	2.238
21 $(C_4H_9)(CH_2=CH)SnCl_2$	54.766	4.122	14.030	3.560	4.875	4.585	6.191	4.982	2.022	0.387	2.370
22 $(C_4H_9)_2SnCl_2$	65.595	6.121	15.764	4.946	5.963	5.193	6.910	5.568	1.597	0.329	3.261
23 $(C_4H_9)_2(CH_2=CH)SnCl$	68.470	5.682	14.306	5.454	6.305	5.403	7.168	5.845	1.719	0.341	3.326
24 $(C_4H_9)_2(CH_2=CH)SnBr$	71.454	5.682	17.090	5.470	6.565	5.408	7.168	6.848	1.719	0.541	5.628
25 $(CH_3)_2(CH_2=CH)_2Sn$	44.238	5.121	11.398	2.943	3.645	3.784	5.235	4.266	1.668	0.393	2.580
26 $(CH_3)_2(C_2H_5)SnI$	49.374	2.561	18.291	2.867	3.501	3.332	4.667	3.798	1.569	0.384	2.518
27 $(CH_3)_2(C_6H_7)_2Sn$	102.183	5.121	18.866	9.716	9.820	6.904	8.868	7.130	1.236	0.210	4.647
28 $(C_2H_5)(C_4H_9)_3Sn$	83.047	7.243	15.315	7.735	7.821	5.992	7.653	5.267	1.273	0.229	4.281
29 $(CH_3)(C_4H_9)_3Sn$	78.600	6.682	15.591	7.226	7.320	5.838	7.680	6.309	1.284	0.235	4.176
30 $(C_3H_7)(C_5H_{11})_3Sn$	101.558	9.243	17.315	9.735	9.821	6.672	8.374	5.487	1.236	0.210	4.674
31 $(C_7H_{15})_4Sn$	147.484	14.243	22.315	14.735	14.821	7.897	10.031	8.456	1.167	0.180	5.309
32 $(C_8H_{13})_4Sn$	128.834	12.243	20.315	12.735	12.821	7.459	9.542	8.026	1.191	0.190	5.076
33 $(CH_3)_2(CH_2=CH)SnBr$	45.808	2.561	15.640	2.456	3.352	3.332	4.667	3.798	1.872	0.479	2.035

Table 2 (continued)

Compounds	<i>MR</i>	$^1X$	$^1X^v$	$^1X^r$	$^1X^b$	$\ln W$	$\ln I_D^w$	$\bar{I}_D^w$	<i>IC</i>	<i>SIC</i>	<i>CIC</i>
34 $(C_4H_9)_2Sn(CH_2CH=CH_2)_2$	84.051	7.243	14.534	6.954	7.647	5.971	7.849	6.537	1.598	0.295	3.828
35 $(Ph_2Sn-(CH_2-CH-CH_2)_2)$	95.900	9.332	13.552	7.082	9.134	6.468	8.449	7.255	1.812	0.343	3.473
36 $Ph_2Sn-(C_4H_9)_2$	105.385	10.332	15.333	8.863	10.308	6.762	8.783	7.547	1.792	0.319	3.823
37 $(CH_3)_2(CH_2=CH)SnI$	34.183	2.561	17.557	2.481	3.414	3.332	4.667	3.798	1.872	0.479	2.035
38 $(CH_3)(C_2H_5)(C_3H_7)SnI$	58.728	3.621	18.516	3.877	4.502	4.205	5.742	4.650	1.562	0.345	2.961
39 $Ph_2Sn(CH_2=CH_2)_2$	83.279	8.332	11.865	6.091	8.134	6.163	8.096	6.910	1.680	0.333	3.364
40 $(Ph-C\equiv C)Sn(CH_3)_3$	65.423	5.578	14.150	4.770	5.952	5.380	7.142	5.825	1.944	0.414	2.756
41 $[(C_2H_5)_3-Sn]_2O$	90.951	7.071	21.211	7.643	8.214	5.864	7.745	6.560	1.487	0.271	4.005
42 $[(C_4H_9)_3-Sn]_2O$	146.594	13.071	27.211	14.214	13.643	7.498	9.612	8.284	1.360	0.215	4.979
43 $(CH_3)_3Sn-OC_4H_9$	51.029	4.061	13.427	4.283	4.776	4.644	6.245	4.955	1.605	0.338	3.150
44 $(C_3H_7)_3Sn-OPh$	86.376	8.260	14.221	7.432	8.528	6.265	8.198	6.906	1.843	0.340	3.583
45 $(C_4H_9)_3Sn-OCH_3$	79.461	7.243	14.014	7.222	7.764	5.992	7.868	6.527	1.481	0.270	4.011
46 $(C_4H_9)_3Sn-OC_4H_9$	99.259	8.743	15.601	8.812	9.279	6.500	8.456	7.070	1.455	0.253	4.300
47 $(C_4H_9)_3Sn-OPh$	99.375	9.760	15.721	8.932	10.028	6.731	8.731	7.387	1.760	0.309	3.940

It can be seen that of the first eight parameters  $^1X$  has the best linear correlation with *MR* for both "ionic" series and covalent series, MCI took advantage over the Wiener information series (*W*,  $I_D^w$ , and  $\bar{I}_D^w$ ) and information content series (*IC*, *SIC* and *CIC*).  $^1X^v$  gave poorer correlation than that of  $^1X$  for both series, especially for the structurally-complicated  $R_mSnX_{4-m}$  ( $m=3,2$ ) series. Hence, the use of valence connectivity index based on  $\delta^v$  conception is not suitable for structure expression of elemental organic compounds.

Table 3 Correlation coefficients of MR and topological indices

Index	Compounds		
	47 $R_mSnX_{4-m}$ ( $m=4,3,2$ )	16 $R_mSnX_{4-m}$ ( $m=3,2$ )	31 $R_4Sn$
<i>IC</i>	0.513	0.594	0.440
<i>SIC</i>	0.735	0.850	0.699
<i>CIC</i>	0.886	0.931	0.886
$\ln W$	0.917	0.929	0.917
$\ln I_D^w$	0.910	0.927	0.999
$\bar{I}_D^w$	0.905	0.944	0.898
$^1X$	0.993	0.978	0.991
$^1X^v$	0.800	0.583	0.930
$^1X^b$	0.997	0.989	0.999
$^1X^r$	0.994	0.990	0.993

Lately, Kupchik obtained the similar conclusion as us in his QSPR studies for alkylger-

manes and alkylsilanes (Kupchik, 1986;1988). He defined two new empirically-modified first order  $MCI_s$ , which we named as radius-corrected  $MCI^1X^r$  (Equation 11) and bond-length-corrected  $MCI^1X^b$  (Equation 13), respectively.

$${}^1X^r = \sum (\delta_i^r \delta_j^r)^{-1/2}, \quad (11)$$

$$\delta^r = r_c/r(Z^v - h), \quad (12)$$

where the meaning of  $Z^v$  and  $h$  is the same as described above,  $r_c$  is covalent radius of carbon,  $r$  is the covalent radius of heteroatom. The  $r$  and  $r_c/r$  values of atoms involved in this paper are listed in Table 4.

$${}^1X^b = \sum b(\delta_i \delta_j)^{-1/2}, \quad (13)$$

where  $\delta$  has the same meaning as described above,  $b$  is the ratio of bond length of the studied edge in molecular graph with that of C-C bond. Bond length and  $b$  values involved in this paper are shown in Table 5.

Table 4  $r$  and  $r_c/c$  values of atoms

Atom	$r$	$r_c/c$	Atom	$r$	$r_c/c$
C	0.77	1.000	Cl	0.99	0.778
Sn	1.40	0.550	Br	1.14	0.676
O	0.74	1.041	I	1.33	0.579
N	0.74	1.041			

Table 5 Bond length and  $b$  values

Chemical bond	Length	$b$	Chemical bond	Length	$b$
C-C	1.54	1.000	C=C(aromatic)	1.39	0.903
C-Sn	2.17	1.409	Sn-O	2.14	1.389
C-O	1.43	0.928	Sn-Cl	2.39	1.552
C=C(alkyl)	1.35	0.877	Sn-Br	2.54	1.649
C≡C	1.20	0.779	Sn-I	2.73	1.772

This paper applied  ${}^1X^b$  and  ${}^1X^r$  in QSPR studies for the 47 structurally-complicated organotins (Table 2). Correlation coefficients of  ${}^1X^r$ ,  ${}^1X^b$  and  $MR$  are shown in Table 3. The improvement of correlation was significant by the use of  ${}^1X^r$  and  ${}^1X^b$  instead of  ${}^1X^v$  for both "ionic" series and covalent series, especially for structurally-complicated "ionic" series which included more heteroatoms. However, when  ${}^1X$  was replaced by  ${}^1X^r$  and  ${}^1X^b$ , the correlation was improved only for structurally-complicated "ionic" series. But it is just these structurally-complicated "ionic" organotins that cause environmental problem and engender the interest of QSA(P)R study. Hence,  ${}^1X^b$  and  ${}^1X^r$  possessed superiority to  ${}^1X$ , especially to  ${}^1X^v$  as steric parameters in QSA(P)R studies of structurally-complicated elemental organic compounds. We recommend  ${}^1X^b$  and  ${}^1X^r$  as primary steric parameters for further studies.

## 4 Conclusion

According to the correlation studies of MR and three catalogs of topological indices for 47 structurally-complicated organotin compounds, *MCI*s were more suitable than Wiener information indices ( $W$ ,  $I_D^w$  and  $\bar{I}_D^w$ ) and information content indices ( $IC$ ,  $CIC$  and  $SIC$ ) for structure expression of structurally-complicated elemental organic compounds. Among *MCI*s, the corrected pattern-valence  $MCI$   $^1X^v$ , which had been proved to be more suitable for structure expression of unsaturation and heteroatoms, failed. The use of two new corrected patterns-radius-corrected  $MCI$   $^1X^r$  and bond-length-corrected  $MCI$   $^1X^b$  improved correlation for both "ionic" series and covalent series. Hence,  $^1X^b$  and  $^1X^r$  possessed superiority to  $^1X$ , especially to  $^1X^v$  as steric parameters in QSA (P)R studies of structurally-complicated elemental organic compounds, and were recommended as primary parameters for further studies.

## References

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