Algorithmically Compressed Data and the Topological Conjecture for the Inner-Core Electrons

Lionello Pogliani†

Dipartimento di Chimica, Università della Calabria, 87030 Rende (CS), Italy

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Eight different properties of three classes of compounds, metal halides, halomethanes, and chlorofluorocarbons, have been modeled with the aim to check the validity of the odd complete graph conjecture suggested for encoding the contribution of the inner-core electrons to the molecular connectivity indices. Modeling using this conjecture is compared with modeling using connectivity indices derived by other well-known algorithms. The conjecture of odd complete graph for the inner-core electrons achieves to improve the modeling quality of the molecular connectivity indices and/or of the molecular connectivity terms. The importance of the recently introduced dual molecular connectivity indices and pseudoindices in further refining the modeling quality of the higher-order terms has also been stressed.

INTRODUCTION

It has been said[1] that **w**hat is new or different about modern science is the nature of its representations. The graph representation, widely used in computational chemistry,[2−8] uses quite simple tools to encode the structure of a molecule, with the aim to derive, among other things, quantitative structure−activity or structure−property relationships (QSAR/QSPR), and to compress a vast amounts of data into simple algorithms.

Molecular connectivity and its "side-branch" the electrotopological state concept[9,10] allow for the use also of a pseudograph representation of molecules to encode multiple bonds and nonbonding electrons. Actually, molecular connectivity uses also atomic concepts, like atomic number, valence electrons, and principal quantum number, to encode the contribution of the inner-core electrons of the higher-row atoms (n > 2) of a molecule. Among the interesting developments that molecular connectivity has undergone recently with the introduction of edge-connectivity indices, line-graph indices, variable descriptors, molecular pseudoconnectivity indices, higher-order connectivity-pseudoconnectivity terms, and finally the dual indices,[11−20] there is none that has achieved in solving the intermingling of graph and atomic concepts that plagues molecular connectivity. Aim of the present study is to propose a solution for this "state of affairs" with the introduction of odd complete graphs to "graph" encode the inner-core electrons of any atom of a molecule whose principal quantum number, n, is equal to or greater than two. For this reason the modeling will here be centered on different physicochemical properties of metal halides, halomethanes, and haloethanes. These classes of compounds have, recently, been the object of many studies.[21,12,22,14,10] The choice of complete graphs goes back to a recent study[23] where their importance was first detected.

† Corresponding author fax: +39-984-492105; e-mail: lionp@unical.it.

METHOD

The Basis Indices. The linear relation used to model a property with a graph-structural descriptor, S, can be written as a dot product: $P = \boldsymbol{C}\cdot S$, where $\boldsymbol{C} = (c_1, c_2, ..., c_0)$, and $S = (S_1, S_2, ..., U_0)$, or as a sum: $P = \Sigma c_i S_i$. Here, c_i and S_i are the single regression parameters and the single structural descriptors, respectively, of the linear or multilinear regression, and $U_0 \equiv 1$. and To avoid negative calculated P values that have no physical or biological meaning it is advantageous to use the modulus equation: $P = |\Sigma c_i S_i,|$, where bars stand for absolute value. Here we will be interested only with structural descriptors, S_i, that can be derived with the molecular connectivity theory. The basis descriptors of this theory, β, are the molecular connectivity and pseudoconnectivity indices, χ and ψ, respectively, supplemented by the corresponding dual and soft dual basis indices, β_d.[20]

$$\{\beta\} = \{\{\chi\}\{\psi\}\{\beta_d\}\} \tag{1}$$

where

$$\{\chi\} = \{D, {}^0\chi, {}^1\chi, \chi_t, D^v, {}^0\chi^v, {}^1\chi^v, \chi^v{}_t\},\ \{\psi\} = \{{}^S\psi_I, {}^0\psi_I, {}^1\psi_I, {}^T\psi_I, {}^S\psi_E, {}^0\psi_E, {}^1\psi_E, {}^T\psi_E\}$$

$$\{\beta_d\} = \{{}^0\chi_d, {}^1\chi_d, {}^1\chi_s, {}^0\chi^v{}_d, {}^1\chi^v{}_d, {}^1\chi^v{}_s, {}^0\psi_{Id}, {}^1\psi_{Id}, {}^1\psi_{Is}, {}^0\psi_{Ed}, {}^1\psi_{Ed}, {}^1\psi_{Es}\}$$

The dual indices of the other basis indices of subsets $\{\chi\}$ and $\{\psi\}$ are redundant, as they differ only by a constant term. The indices $\{\chi\}$ and $\{\psi\}$ are defined in the following way[9,12−14]

$$D = \Sigma_i \delta_i \tag{2}$$

$${}^S\psi_I = \Sigma_i I_i \tag{3}$$

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$$^0\chi = \Sigma_i(\delta_i)^{-0.5} \quad (4)$$

$$^0\psi_I = \Sigma_i(I_i)^{-0.5} \quad (5)$$

$$^1\chi = \Sigma(\delta_i\delta_j)^{-0.5} \quad (6)$$

$$^1\psi_I = \Sigma(I_iI_j)^{-0.5} \quad (7)$$

$$\chi_t = (\delta_1\cdot\delta_2\cdot\delta_3\cdot.....\cdot\delta_N)^{-0.5} = (\Pi\delta_i)^{-0.5} \quad (8)$$

$$^T\psi_I = (I_1\cdot I_2\cdot I_3\cdot.....\cdot I_N)^{-0.5} = (\Pi I_i)^{-0.5} \quad (9)$$

The index χ_t (and χ^v_t) is the total molecular connectivity index, and it has its ψ counterpart in the total molecular pseudoconnectivity index, $^T\psi_I$ (and $^T\psi_E$). The sums in eqs 2−5 as well as products (Π) in eqs 8 and 9 are taken over all vertices of the hydrogen-suppressed chemical graph. The sums in eqs 6 and 7 are taken over all edges of the chemical graph (σ bonds in a molecule). Replacing in eqs 2, 4, 6, and 8, δ with δ^v gives the subset of valence χ^v indices, $\{D^v, {}^0\chi^v, {}^1\chi^v, \chi^v_t\}$, where superscript v stands for valence. Replacing I_i with S_i in eqs 3, 5, 7, and 9 gives the pseudoconnectivity electrotopological (E) ψ_E subset $\{{}^S\psi_E, {}^0\psi_E, {}^1\psi_E, {}^T\psi_E\}$. The superscripts S and T stand for sum and total, the other superscripts follow the established denomination for χ indices.[9] The dual indices, $\{\beta_d\}$, are defined in the following way (subscript *d* stands for dual and *s* for soft dual)[20]

$$^0\chi_d = (-0.5)^N\Pi_i(\delta_i) \quad (10)$$

$$^0\psi_{Id} = (-0.5)^N\Pi_i(I_i) \quad (11)$$

$$^1\chi_d = (-0.5)^{(N+\mu-1)}\Pi(\delta_i + \delta_j) \quad (12)$$

$$^1\psi_{Id} = (-0.5)^{(N+\mu-1)}\Pi(I_i + I_j) \quad (13)$$

$$^1\chi_s = \Pi(\delta_i + \delta_j)^{-0.5} \quad (14)$$

$$^1\psi_{Is} = \Pi(I_i + I_j)^{-0.5} \quad (15)$$

In the same way the subsets of dual valence χ^v_d indices and dual ψ_{Ed} indices are defined. In the first case δ^v replaces δ in eqs 10, 12, and 14, while in the second case S_i replaces I_i in eqs 11, 13, and 15. The exponent μ of eqs 12 and 13 is the cyclomatic number. This number is a molecular descriptor[6] that indicates the number of bonds that must be broken in order to obtain a cycle-free structure. Removing an edge is equivalent to opening a ring by breaking a bond in the ring. For acyclic molecules $\mu = 0$, for monocyclic compounds $\mu = 1$, and for bicyclic compounds $\mu = 2$. From these equations, it can be noticed that the dual indices, $^0\chi_d$ and $^0\chi^v_d$, $^1\chi_d$, and $^1\chi^v_d$ as well as $^0\psi_{Id}$ and $^0\psi_{Ed}$, $^1\psi_{Id}$ and $^1\psi_{Ed}$ can have, depending on the number of vertices of the chemical graph, negative values, and that $^1\chi^v_d$ and, especially, the rescaled (see later on) $^1\psi_{Ed}$ index can assume quite large values even for rather small compounds. From the definitions of the soft dual indices we note that they are always positive and span a smaller range of values. The factor $(-0.5)^N$ is not constant throughout classes of nonisomeric compounds as it depends on N, and in this case, the dual indices, $^0\chi_d$, $^0\chi^v_d$, $^0\psi_{Id}$, and $^0\psi_{Ed}$ are not related to the total indices, χ_t, χ^v_t, $^T\psi_I$, and $^T\psi_E$.

The easiest way to avoid the huge combinatorial problem generated by 28 indices (with 25 indices 33 554 431 different combinations are possible[12]) is to use the dual indices at the level of a CI-GTBI, as explained later on. With isomeric and isocyclomatic classes of compounds the factors $(-0.5)^N$ and $(-0.5)^{N+\mu-1}$ are constant, and the zeroth-order dual indices as well as the zeroth-order dual pseudoindices are then related to the corresponding total indices

$$^0\chi_d = \text{const}\cdot(\chi_t)^{-2};\ ^0\chi^v_d = \text{const}\cdot(\chi^v_t)^{-2};\ ^0\psi_{Id} = \text{const}\cdot(^T\psi_I)^{-2};\ ^0\psi_{Ed} = \text{const}\cdot(^T\psi_E)^{-2} \quad (16)$$

For deceptively simple graphs made up of two connected points, ●−● (here, $\chi_t \equiv {}^1\chi$, and so on), the zeroth-order dual index and the first-order dual and soft dual indices obey the following relations[20]

$$^0\chi_d = (-0.5)^2\cdot(\delta_1\cdot\delta_2) = 0.25\cdot(\chi_t)^{-2};\ ^0\chi^v_d = 0.25\cdot(\chi^v_t)^{-2};\ ^0\psi_{Id} = 0.25\cdot(^T\psi_I)^{-2};\ ^0\psi_{Ed} = 0.25\cdot(^T\psi_E)^{-2};\ ^1\chi_d = (-0.5)\cdot(\delta_1 + \delta_2) = -0.5\cdot D;\ ^1\chi^v_d = -0.5\cdot D^v;\ ^1\psi_{Id} = -0.5\cdot{}^S\psi_I;\ ^1\psi_{Ed} = -0.5\cdot{}^S\psi_E;\ ^1\chi_s = (\delta_1 + \delta_2)^{-1/2} = D^{-1/2};\ ^1\psi_{Es} = (^S\psi_E)^{-1/2} \quad (17)$$

In this case dual and soft dual indices are related.

The Rationale of Basis Indices. Basis χ indices and valence χ^v indices are directly based on the δ and δ^v connectivity numbers of a hydrogen-suppressed graph and pseudograph, respectively.[9,12] If the molecule does not contain any higher-row atoms, i.e., atoms with principal quantum number n > 2, then δ and δ^v values can be derived from the corresponding chemical graph and pseudograph of a hydrogen-suppressed molecule, respectively. The δ^v values for higher-row atoms (n > 2, here: Na, K, Rb, Cs, Mg, Ca, Sr, Cl, Br, and I) can be obtained by the aid of the following algorithm[9]

$$\delta^v = [Z^v - h]/[Z - Z^v - 1] \quad (18)$$

Here, Z^v = number of valence electrons, Z = atomic number, and h = number of suppressed hydrogen atoms. For n = 2 and h = 0, $\delta^v = Z^v$, as, in this case, $Z = Z^v + 2$. The hydrogen-suppressed pseudograph of a molecule allows self-connections (or loops) that count twice and also multiple connections[12] that model nonbonding electrons and multiple bonds. A pseudograph thus has a wider applicability than the corresponding graph, which allows only single connections thereby encoding only the σ molecular framework. Thus, while the hydrogen-suppressed graph of CH_3F can be represented by two connected points, ●−●, where each vertex has $\delta = 1$, the hydrogen-suppressed pseudograph of CH_3F is shown in Figure 1, overlooking, for the moment being, what is shown in the inner-circle. Here, the first vertex that represents C has $\delta^v = 1 = \delta$, while the fluorine vertex has $\delta^v = 7$ (each loop counts twice, plus the single-connection). Equation 18 tells us that only second-row atoms can be encoded by the aid of graph-theoretical concepts only.

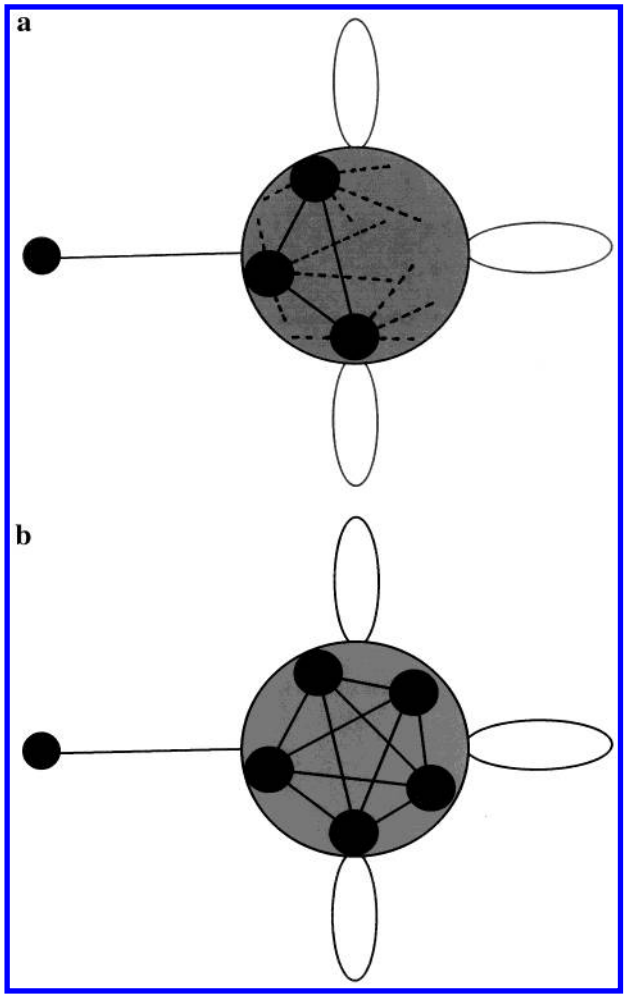

Figure 1. a. A nonspecific hydrogen-suppressed pseudograph of a CH_3-X compound, with a blow-up of the X vertex, which shows an odd complete graph for the inner-core electrons of an undefined halogen atom, X. Inner-core electrons of carbon atom are encoded by a K_1 graph. b. The hydrogen suppressed pseudograph of CH_3-Br, with a blow-up of the Br vertex, which shows a K_5 complete graph to encode the inner-core electrons of Br.

Basis ψ indices are indirectly related to δ and δ^v numbers through the intrinsic I-state (ψ_I subset) and the electrotopological S-state (ψ_E subset) atom level indices,[10] which are defined in eqs 19 and 20

$$I_i = [(2/n)^2\delta_i{}^v + 1]/\delta_i \tag{19}$$

$$S_i = I_i + \Sigma_j \Delta I_{ij} \tag{20}$$

The intrinsic state index encodes the availability of the atom or group for intermolecular interaction and the manifold of bonds over which adjacent atoms may influence, and be influenced by, its state. The electrotopological state index takes into account the actual state of an atom in a molecule plus the influence of all other atoms in the molecule, which is included in $\Sigma_j\Delta I_{ij}$. The $\delta_i{}^v$ parameter of the I-state index can be derived from the pseudograph (ps) of a molecule, i.e, $\delta_i{}^v = \delta_i{}^v(ps)$. The inner-core electron contribution for higher-row atoms (n > 2) is encoded by the $(2/n)^2$ factor only, i.e., $\delta^v(F) = \delta^v(ps)$, $\delta^v(Cl) = (2/3)^2\delta^v(ps)$, $\delta^v(Na) = (2/3)^2\delta^v(ps)$, $\delta^v(I) = (2/5)^2\delta^v(ps)$, and so on, where $\delta^v(ps)$-[F, Cl, Br, I] = 7, and $\delta^v(ps)$[Li, Na, K, ...] = 1. Equation 19 could be rewritten as follows: $I_i = [\delta_i{}^v+1]/\delta_i$ where, $\delta_i{}^v = (2/n)^2\delta_i{}^v(ps)$. From this follows that χ^v and ψ indices are based on different δ^v definitions, i.e., $\delta^v = [Z^v-h]/[Z-Z^v-1]$ and $\delta^v = (2/n)^2\delta^v(ps)$, and only for $n = 2$ the two definitions coincide. This means that a description based on χ^v and ψ indices, for higher-row atoms, has a heterogeneous character. As the choice $\delta_i{}^v = (2/n)^2\delta_i{}^v(ps)$ seems optimal for the electrotopological state,[10] the possibility of a so-called homogeneous description remains, where $\chi^v = f[(2/n)^2\delta_i{}^v(ps)]$.

In eq 20 the factor ΔI_{ij} equals $(I_i-I_j)/r^2_{ij}$, where r_{ij} counts the atoms in the minimum path length separating two atoms i and j, which equals the graph distance, $d_{ij} + 1$. As highly electropositive atoms have negative *S* values,[10] to avoid imaginary ψ_E values, a rescaling procedure is mandatory.[13,14] In this study, S for metal halides, MeHal, has been rescaled to the *S* value of Ba in BaF_2, where $S[Ba(BaF_2)] = -3.083$, S for the halomethanes has been rescaled to the *S* value of Si in SiF_4, where, $S[Si(SiF_4)] = -6.611$, and S for the chlorofluorocarbons has been rescaled to $S[C(CF_4)] = -5.5$. The rescaling invalidates an important result of the I_S concept,[10] with the consequence that $\Sigma S_i \neq \Sigma I_i$ and ${}^S\psi_I \neq {}^S\psi_E$. Normally $\Sigma S_i = \Sigma_i I_i$ holds and consequently, ${}^S\psi_I = {}^S\psi_E$, and in this case the ψ-subset consists of seven indices only.

The K_p-Odd-Complete-Graphs. The problem of encoding the inner-core electrons of atoms with $n \geq 2$ by the aid of a graph representation could elegantly be solved by the aid of complete graphs and especially of K_p-odd-complete-graphs. If recent results on this topic[23] are confirmed then, the graph representation of a hydrogen-suppressed molecule could be complete. Let us first spend some words about complete graphs to understand what a K_p-odd-complete-graph is. A graph G is complete if every two of its vertices are adjacent. A complete graph of order *p* is denoted by K_p and is *r*-regular ($p - 1 = r$), where *r* is its regularity, if it has all vertices with the same degree, where the degree of a vertex is the number of edges incident with it. The *p* values here used are as follows: $p = 1$ ($r = 0$) for the second-row atoms, $p = 3$ ($r = 2$) for the third-row atoms, $p = 5$ ($r = 4$) for the fourth-row atoms, and $p = 7$ ($r = 6$) for fifth-row atoms, and so on. In Figure 1A,B is shown the hydrogen-suppressed pseudograph (ps) together with a zoom of a generic K_p (1A) and K_5 (1B) odd complete graph that encode the inner-core electrons of X (1A) and of Br (1B) of a CH_3-X and CH_3-Br compound. The algorithm chosen to derive δ^v by the aid of the K_p-odd-graphs plus the (external) pseudograph is

$$\delta^v = \delta^v(ps)/[p\cdot r+1] \tag{21}$$

A clue for this choice is given by eq 18, where the halogen atoms along the series, CH_3-F, CH_3-Cl, CH_3-Br, and CH_3-I, have $\delta^v = 7/1$ for F, $\delta^v = 7/9$ for Cl, $\delta^v = 7/27$ for Br, and $\delta^v = 7/45$ for I. Here the numerator can be derived by the aid of the corresponding hydrogen-suppressed pseudograph (ps), and the denominator can fairly be approximated by the following: $1 = (n-1)^2$ for F, $9 = 3^2 = n^2$ for Cl, $27 \approx 5^2 = (n+1)^2$ for Br, and $45 \approx 7^2 = (n+2)^2$ for I. That is, if the *p* values are odd, i.e., 1, 3, 5, and 7, algorithm 21 will allow to derive δ^v values (7/1, 7/7, 7/21, 7/43), not tremendously far from the old values, and that could compete with them. The choice of even complete graphs would oblige to start with a $p = 2$ complete graph for the every second row atom (unless to define a rather

strange complete $p = 0$ graph), invalidating the regular method used to model second-row atoms in chemical graphs, i.e., with vertices. These vertices, in fact, can, practically, be thought of as K_1 odd complete graphs, with the advantage that for $n = 2$, $\delta^v \equiv \delta^v(ps)$ or δ (for simple graphs).

It is well-known that δ and δ^v values can be obtained by the aid of the adjacency matrix either of a graph[9] or of a pseudograph,[12] respectively. Actually it is possible to obtain both δ and δ^v values from the adjacency matrix of a pseudograph, as a graph is a special case of pseudograph.[12] The adjacency matrix of a hydrogen-suppressed pseudograph of a triatomic system inclusive of its K_p-odd-complete-graph is

$$A = (p \cdot r + 1)^{-1}{}_{Kp} \begin{pmatrix} ps_{1,1} & g_{1,2} & g_{1,3} \\ g_{2,1} & ps_{2,2} & g_{2,3} \\ g_{3,1} & g_{3,2} & ps_{3,3} \end{pmatrix} \qquad (22)$$

Here, $g_{i,j}$ can be either 0 or 1. It is one only if vertices i and j are connected, otherwise it is zero; $ps_{i,i}$ is the sum of the self-connections (they count twice) and multiple connections of vertex i (pseudograph characteristics only, ps). The factor $(p \cdot r + 1)^{-1}{}_{Kp}$ encodes the odd-complete-graph characteristics and depends on the p value of each vertex. I.e. the adjacency matrix for the pseudograph-K_p-odd-complete-graph of CH_2O (K_1 for both C and O), CH_3-I (K_1 for C, and K_7 for I), and MgF_2 (K_1 for F, and K_3 for Mg) are (numbering indicates the row)

$$A(C_1O_2) = \begin{pmatrix} 1/1 & 1/1 \\ 1/1 & 5/1 \end{pmatrix}, A(C_1I_2) = \begin{pmatrix} 0 & 1/1 \\ 1/43 & 6/43 \end{pmatrix},$$

$$A(F_1Mg_2F_3) = \begin{pmatrix} 6/1 & 1/1 & 0 \\ 1/7 & 0 & 1/7 \\ 0 & 1/1 & 6/1 \end{pmatrix}$$

Clearly, now, the adjacency matrices are asymmetric.

The Configuration Interaction of Graph-Type Basis Indices (CI-GTBI). To further improve the modeling quality and avoid as much as possible a series of problems that normally arise with linear combinations of basis indices (LCBI), index-interrelation, overfitting, chance correlation, ..., it is advantageous to work, whenever possible, with a modeling equation based on a single powerful structural descriptor, $P = c_1S + c_0U_0$. Quantum methods, like the linear combinations of Gaussians-type orbitals and configuration interaction methods, give us a hint how to derive such powerful descriptors, which have been called either terms or configuration interaction of graph type basis indices (CI-GTBI). Three types of terms will be used: X, Y, and the higher-order mixed term, Z, where $X = f(\chi)$, $Y = f(\psi)$, and $Z = f(X,Y)$ or $f(X, Y, \beta)$, where $\beta = \chi$ or ψ.[12-14,19] To avoid a huge combinatorial problem the dual indices are introduced at this level, and they normally give rise to $Z' = f(X,Y, \beta_d)$ or $f(X, Y, \beta, \beta_d)$ terms.[20] While the procedure to choose the best basis indices of a LCBI is a search procedure performed on the total combinatorial space described by the basis indices $\{\beta\}$, the procedure used to construct the dominant molecular connectivity terms, X, and Y is a trial-and-error procedure[12] that chooses the basis indices optimizing, then, a series of adjustable parameters. Terms X and Y look like the rational function of eq 23, where β is a basis index, and $S = X$ or Y for $\beta = \chi$ or $\beta = \psi$, respectively. The optimization parameters $a-d$, $m-r$ can be either negative, zero, or one

$$S = [a(\beta_1)^m + b(\beta_2)^n]^q/[c(\beta_3)^o + d(\beta_1)^p]^r \qquad (23)$$

The Z terms are derived with a procedure that tries different ways to combine terms X and Y together.[14,19] This procedure will also be called a trial-and-error search for terms.[20] The CI-GTBI allows bypassing the combinatorial problem performed on a set of 16 basis indices made up of eight χ and eight ψ indices if ${}^S\psi_I \neq {}^S\psi_E$ and 15 if ${}^S\psi_I = {}^S\psi_E$.

The statistical performance of the graph-structural molecular connectivity invariant, S, is controlled by a quality factor, $Q = r/s$, and by the ratio $F = fr^2/[(1-r^2)\nu]$, where r and s are the correlation coefficient and the standard deviation of the estimates, respectively, f is the number of freedom degrees $= n-(\nu+1)$, ν is the number of variables, and n is the number of data. The parameter Q has no absolute meaning as it is an "intra" statistical parameter, which is able to compare only the descriptive power of different descriptors for the same property.[24] The F ratio, a kind of "inter" statistical parameter, tells us, even if Q improves, which additional descriptor endangers the quality of the modeling. For every structural descriptor, be it a basis index, a LCBI, a term and the unitary descriptor, U_0, the fractional utility, $u_i = |c_i/s_i|$, where s_i is the confidence interval of c_i, and the average fractional utility $\langle u \rangle = \Sigma u_i/(\nu+1)$ will be given. If the modeling relation is linear, then $\langle u \rangle = (u_1+u_0)/2$. The utility statistics allows us to detect descriptors that give rise to unreliable coefficient values (c_i), whenever their deviation interval (s_i) is high. This statistic allows for detection of the paradoxical situation of good predictive equations with bad utility.[25,12] In modeling studies the value of the standard deviation of the estimate s is critical,[20] thus, to have a direct idea of how much this statistic improves along a series of descriptors, the ratio $s_R = s_0/s_i$ is introduced here, where s_0 is the s value of the best single-index description and s_i refers to the s values of the improved sequential descriptions, that sometimes shows an improved r but a worse s. We underline then, that (i) all statistical parameters will now grow with improving modeling and that (ii) every modeling will be under the control of all of these statistics, and that (iii) nothing justifies that an improved Q is a good receipt for a good modeling. The richness in statistical parameters can also be used to detect eventual printing errors, as redundancy is very useful in the construction of self-correcting codes. To avoid to bother the reader with the dimensional problems of P in the modeling equations, every property P should be read as P/P° where P° is the unitary value of the property.

RESULTS AND DISCUSSION

Methal Halides, MeHal. Concerning the possibility to represent inorganic salts with a graph or a pseudograph the reader is referred to papers 12, 26, and 27 where interesting considerations are drawn about purely ionic and purely covalent bonds in these compounds. The lattice enthalpy, $\Delta H_L^\varnothing$ (kJ mol^{-1}), of metal halides, MeHal, at 298.15 K, together with the corresponding molecular connectivity and pseudoconnectivity values are collected in Tables 1 and 2. The valence molecular connectivity values are those obtained by encoding the inner-core electrons of Me and Hal with the K_p graphs, where p = 1, 3, 5, 7, and 9 for $n = 2$, 3, 4,

Table 1. Lattice Enthalpies, $\Delta H_L^{\varnothing}$ (kJ mol^{-1}), at 298.15 K, Corresponding Calculated Values, $\Delta H_L^{\varnothing}$(C), Percent Residual, Δ%, Molar Masses, M, and Odd-K_p-Graph Valence Molecular Connectivity Indices for 20 MeHal Metal Halides

MeHal	$\Delta H_L^{\varnothing}$	$\Delta H_L^{\varnothing}$(C)	Δ%	M	D^v	$^0\chi^v$	$^1\chi^v$
LiF	1037	1038	0.06	25.94	8	1.37796	0.37796
NaF	926	903	2.5	41.99	7.14	3.05058	1.01015
KF	821	836	1.9	50.10	7.048	4.94232	1.72516
RbF	789	796	0.9	104.47	7.023	6.97177	2.49222
CsF	750	772	2.9	151.90	7.014	8.82951	3.19438
LiCl	852	874	2.6	42.39	2	2	1
NaCl	786	764	2.7	58.44	1.143	3.64443	2.64443
KCl	717	723	0.9	74.55	1.048	5.56435	4.56435
RbCl	695	700	0.8	120.92	1.023	7.59380	6.59380
CsCl	678	686	1.2	168.36	1.014	9.45154	8.45154
LiBr	815	804	1.3	86.85	1.333	2.73292	1.73292
NaBr	752	709	5.7	102.89	0.476	4.37735	4.58258
KBr	689	679	1.5	119.00	0.381	6.29727	7.90965
RbBr	668	663	0.7	165.37	0.356	8.32672	11.4265
CsBr	654	654	0.04	212.81	0.347	10.1845	14.6458
LiI	761	770	1.2	133.85	1.163	3.47689	2.47689
NaI	705	684	3.0	149.89	0.306	5.12132	6.54995
KI	649	658	1.3	166.00	0.211	7.04124	11.3054
RbI	632	645	2.0	212.372	0.186	9.07069	16.3321
CsI	620	638	2.8	259.81	0.177	10.9284	20.9335

Table 2. Molecular Pseudoconnectivity, ψ-I$_S$, Indices of 24 Metal Halides[a]

MeHal	$^S\psi_I$	$^0\psi_I$	$^1\psi_I$	$^S\psi_E$	$^0\psi_E$	$^1\psi_E$
LiF	10	1.06066	0.25	16.166	0.81020	0.14893
NaF	9.444	1.18573	0.29422	15.611	0.86870	0.16495
KF	9.25	1.24798	0.31623	15.417	0.89469	0.17205
RbF	9.16	1.28203	0.32827	15.326	0.90791	0.17567
CsF	9.111	1.30228	0.33543	15.277	0.91548	0.17774
LiCl	6.111	1.20031	0.34875	12.277	0.82841	0.16861
NaCl	5.555	1.32538	0.41043	11.722	0.86559	0.18151
KCl	5.361	1.38763	0.44113	11.527	0.88132	0.18694
RbCl	5.271	1.42168	0.45793	11.437	0.88921	0.18966
CsCl	5.222	1.44193	0.46792	11.388	0.89365	0.19118
LiBr	4.75	1.31013	0.42718	10.917	0.85947	0.18418
NaBr	4.194	1.43520	0.50182	10.36	0.89084	0.19659
KBr	4	1.49745	0.53936	10.166	0.90400	0.20174
RbBr	3.91	1.53150	0.55989	10.077	0.91052	0.20428
CsBr	3.861	1.55175	0.57211	10.027	0.91430	0.20574
LiI	4.12	1.39391	0.48564	10.286	0.88201	0.19447
NaI	3.564	1.51898	0.57154	9.731	0.91042	0.20665
KI	3.37	1.58123	0.61430	9.537	0.92240	0.21170
RbI	3.28	1.61528	0.63768	9.446	0.92844	0.21423
CsI	3.231	1.63553	0.65159	9.397	0.93182	0.21565

[a] The rescaling procedure for ψ_E indices has been done on the S[Ba(BaF$_2$)]= −3.083.

5, and 6, respectively. As the graph of metal halides are deceptively simple graphs, actually K_2 graphs: ●−●, the only subsets of meaningful indices are as follows: $\{\chi^v\} = \{D^v, {}^0\chi^v, {}^1\chi^v\}$ and $\{\psi\} = \{{}^S\psi_I, {}^0\psi_I, {}^1\psi_I, {}^S\psi_E, {}^0\psi_E, {}^1\psi_E\}$. The lattice enthalpy of metal halides has already been modeled with $\chi^v = f[Z^v/(Z-Z^v-1)]$ indices.[21,12] The obtained results were

$$\{{}^0\chi^v\}:\ Q = 0.013,\ F = 36,\ r = 0.815,\ s_0 = 62.3,\ n = 20$$

$$X = [(D^v)^{0.5} + 0.2]/[D^v + 4.2\cdot{}^0\chi^v]$$

$$Q = 0.037,\ F = 281,\ r = 0.969,\ s_R = 2.60,\ n = 20,$$
$$\mathbf{u} = (17, 65),\ \langle u\rangle = 41$$

The only χ^v description based on odd complete graphs, which offers a superior alternative to the previous ones is

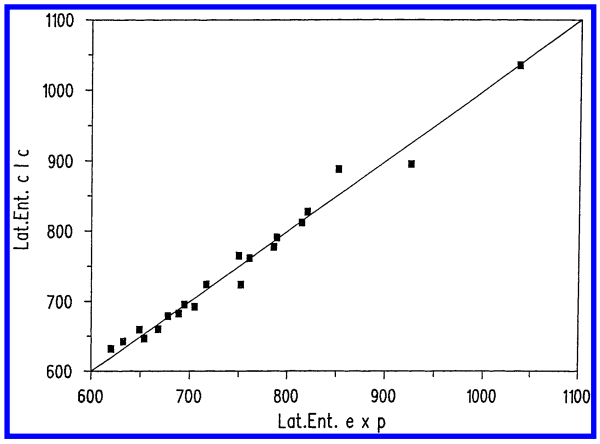

Figure 2. Plot of the calculated lattice enthalpy values vs their corresponding experimental values for 20 metal halides.

the following CI-GTBI, which is the best description for this property

$$X(K_p) = [(D^v)^{0.5}/(D^v + 13.3\cdot({}^0\chi^v)^{0.9}]^{0.6}$$

$$Q = 0.056,\ F = 654,\ r = 0.987,\ s_R = 3.54,\ n = 20,$$
$$\mathbf{u} = (26, 74),\ \langle u\rangle = 50,\ \mathbf{C} = (1730.77, 577.713)$$

Pseudoconnectivity basis indices which, up to now, have never been used with these compounds, provide the single-basis and multi-basis-index descriptions for this property

$$\{{}^0\psi_I\}:\ Q = 0.028,\ F = 159,\ r = 0.948,\ s_R = 1.82,$$
$$\mathbf{u} = (13, 23),\ \langle u\rangle = 19$$

$$\{{}^0\psi_I, {}^1\psi_I\}:\ Q = 0.041,\ F = 170,\ r = 0.976,$$
$$s_R = 2.60,\ \mathbf{u} = (8.2, 4.4, 16),\ \langle u\rangle = 9.7$$

$$\{{}^S\psi_I, {}^0\psi_I, {}^1\psi_I\}:\ Q = 0.062,\ F = 263,\ r = 0.990,$$
$$s_R = 3.87,\ \mathbf{u} = (4.7, 13, 7.8, 20),\ \langle u\rangle = 11$$

$$\mathbf{C} = (23.1614, -1625.86, 1713.29, 1957.71)$$

Figure 2 has been obtained with this last correlation vector, while with the correlation vector of the X(K_p) term, $\mathbf{C}$ = (1730.77, 577.713), the calculated lattice enthalpy values, $\Delta H_L^{\varnothing}$(C), and the percent residual, $\Delta\% = [\Delta H_L^{\varnothing} - \Delta H_L^{\varnothing}\text{-(C)}]\cdot 100/\Delta H_L^{\varnothing}$, shown in Table 1, have been obtained. The last X(K_p) term competes quite effectively at the F and utility level with the $\{{}^S\psi_I, {}^0\psi_I, {}^1\psi_I\}$ combination. No good Y term could be found. An attempt to describe the lattice enthalpy with homogeneous $\chi^v = f[(2/n)^2\delta^v(ps)]$ indices gave results similar to the $\chi^v = f[\delta^v{=}Z^v/(Z-Z^v-1)]$ case for the single-basis and multiple-basis descriptions and poorer results for the X term. Before closing let us rapidly check the descriptive power of the molar mass of these compounds, $\{M\}$: Q = 0.015, F = 43, r = 0.846, s_R = 1.10, and n = 20.

Halomethanes, CH_nX_{4-n}. In the following paragraphs, the modeling of five properties of halomethanes,[26] shown in Table 3, will be undertaken. The corresponding basis descriptors are shown in Tables 4−7. The valence molecular connectivity basis indices, χ^v, have been calculated in three different ways.

Table 3. Physical Properties of Halomethanes, CH_nX_{4-n}: Molar Mass, M/amu, Dipole Moment, μ/D, Molar Refraction, $R_m/cm^3\,mol^{-1}$, Boiling Points, BP/K, Ionization Potential, IP/ev, and Parachor, $\mathscr{P}$[a]

CH_nX_{4-n}	M/amu	μ/D	R_m/cm^3mol^{-1}	BP/K	IP/ev	$\mathscr{P}$[a]
CH_3F	34	1.85	6.7	195	12.85	78
CH_2F_2	52	1.97	6.6	221		87
CHF_3	70	1.65	6.5	189		96
CF_4	88	0	6.4	144		105
CH_3Cl	51	1.87	11.7	249	11.3	
CH_2Cl_2	85	1.80	16.6	313	11.35	
$CHCl_3$	119	1.01	21.5	335	11.4	
CCl_4	154	0	26.4	349	11.4	221
$CFCl_3$	137	0.45	21.4	297	12.9	192
CF_2Cl_2	121	0.51	16.4	243	12.3	163
$CHFCl_2$	102	1.29	16.4	282	12.4	
CHF_2Cl	86	1.42	11.5	233	12.45	
CF_3Cl	104	0.50	11.4	192	11.8	134
CH_2FCl	68	1.82	11.6	264		
CH_3Br	95	1.81	14.6	277	10.5	
CH_2Br_2	174	1.43	22.4	370		
$CHBr_3$	253	0.99	30.2	422		
CBr_4	332	0	38.0	462		277
CF_3Br	149	0.65	14.3	214		
CF_2Br_2	210	0.66	22.2	298		
$CFBr_3$	271	0.58	30.1	381		
CCl_3Br	198	0.21	29.3	378		
CCl_2Br_2	243		32.2	408		
$CClBr_3$	287		35.1	433		
CH_2FBr	113		14.5	291		
CH_2ClBr	129		19.5	342	10.8	
$CHFClBr$	147		19.4	309		
CHF_2Br	131	1.60	14.4	259		
$CHFBr_2$	192		22.3	338		
$CHCl_2Br$	164		24.4	361	10.9	
$CHClBr_2$	208		27.3	394		
$CFCl_2Br$	182		24.3	326		
$CFClBr_2$	226		27.2	353		
CF_2ClBr	165		19.3	269		

[a] The dimensions of $\mathscr{P}$ are not given in the original paper (ref 26), they can be derived from the corresponding equation (see Discussion section).

(1) Odd-K_p-Graph Algorithm for $\delta^v = \delta^v(ps)/(p\cdot r+1)$, Where p = 1 (F), 3 (Cl), 5 (Br), and r = p−1. *Molar Refraction, R_m.* The molar refraction values, $R_m = (M/\rho)\text{-}(n^2-1)/(n^2+2)$, where n is the refractive index, of 34 halomethane are shown in Table 3. To a good approximation molar refractions are the sums of contributions from the individual groups making up a molecule or solid and are nearly independent of temperature. The molar mass, *M*, shown in the same table, is a rather good descriptor for this property, with Q = 0.303, F = 217, r = 0.934, s_R = 0.55, n = 34. The connectivity indices but, especially, the two-ψ-index combination show an optimal modeling power

$$\{{}^0\chi^v\}:\ Q = 0.572,\ F = 773,\ r = 0.980,\ s_0 = 1.71,\ s_R = 1,\ n = 34,\ \mathbf{u} = (28, 1.0),\ \langle u\rangle = 14$$

$$\{{}^S\psi_I,\ {}^1\psi_I\}:\ Q = 4.439,\ F = 23314,\ r = 0.9997,\ s_R = 7.43,\ n = 34,\ \mathbf{u} = (130, 204, 85),\ \langle u\rangle = 139$$

$$\mathbf{C} = (-0.78866,\ 17.07997,\ 10.6894)$$

Note the consistent improvement in every statistic in going from $\{{}^0\chi^v\}$ to $\{{}^S\psi_I,{}^1\psi_I\}$ and in the utility of the unitary descriptor, U_0, from c_0 = 1.0 to c_0 = 85. The interesting X′-type term, where $X = ({}^0\chi^v + \chi_t)^{0.6}$, cannot be compared with the $\{{}^S\psi_I,{}^1\psi_I\}$ combination

$$X' = [X - 10^{-4}\cdot{}^1\chi^v{}_d],\ Q = 0.732,\ F = 1269,\ r = 0.988,\ s_R = 1.27,\ n = 34,\ \mathbf{u} = (36, 18),\ \langle u\rangle = 27$$

Boiling Point, BP. The molar mass, *M*, is a deceiving descriptor for this property, with Q = 0.019, F = 190, r = 0.837, s_R = 0.70, n = 34. The two-mixed-index linear combination shows, instead, an optimal modeling for this property

$$\{{}^1\chi^v\}:\ Q = 0.031,\ F = 190,\ r = 0.925,\ s_0 = 29.9,\ n = 34,\ \mathbf{u} = (14, 10),\ \langle u\rangle = 12$$

$$\{{}^0\chi,\ {}^0\psi_I\}:\ Q = 0.115,\ F = 1319,\ r = 0.994,\ s_R = 3.47,\ n = 34,\ \mathbf{u} = (41, 50, 6.6),\ \langle u\rangle = 33$$

With the boiling points a fine model uses a combination of three basis indices made up of the best combination for R_m, $\{{}^S\psi_I,{}^1\psi_I\}$, and a χ_t basis index

$$\{{}^S\psi_I,\ {}^1\psi_I,\ \chi_t\}:\ Q = 0.183,\ F = 2202,\ r = 0.998,\ s_R = 5.47,\ n = 34,\ \mathbf{u} = (52, 19, 12, 26),\ \langle u\rangle = 27$$

$$\mathbf{C} = (-11.3773,\ 87.2807,\ -227.493,\ 519.035)$$

Comparison with the optimal basis index combination, $\{{}^0\chi,{}^0\psi_I\}$, indicates an interesting improvement in nearly any statistical parameter and especially in the c_0 utility of U_0 (from 6.6 to 41). For the boiling points no optimal CI-GTBI of any type could be found.

Parachor, $\mathscr{P}$. This property, which is also an additive function of atoms and groups in a molecule and is approximately independent of temperature, is a function of the molecular volume with a suitable correction for the cohesive forces of the liquid.[28] The empirical equation $\sigma = M\gamma^{1/4}/(\rho_l-\rho_v)$ shows that the parachor is related to the surface tension γ and to the densities of the liquid and of the vapor, ρ_l and ρ_v, respectively. As expected, the molar mass is a rather good descriptor for this property of nine halomethanes as follows: Q = 0035, F = 46, r = 0.931, s_R = 0.57, and n = 9. The modeling improve with a single valence χ^v index and, especially, with a two-ψ-basis-index descriptor, which is the same descriptor for R_m, and, practically, for BP, if a zero is added in the correlation vector **C** of R_m and $\mathscr{P}$ that zeroes the correlation parameter for χ_t

$$\{{}^0\chi^v\}:\ Q = 0.065,\ F = 157,\ r = 0.978.\ s_0 = 15.1,\ s_R = 1,\ n = 9,\ \mathbf{u} = (13, 4.2),\ \langle u\rangle = 8$$

$$\{{}^S\psi_I,\ {}^1\psi_I\}:\ Q = 0.395,\ F = 2915,\ r = 0.9995,\ s_R = 5.97,\ n = 9,\ \mathbf{u} = (31, 73, 28),\ \langle u\rangle = 44$$

$$\mathbf{C} = (-3.6285,\ 110.4638,\ 86.86556)$$

A trial-and-error procedure discovers the following X′-type CI-GTBI but neither an Y-type term nor a Z-type term.

Table 4. Molecular Connectivity Indices for Halomethanes[a]

CH_nX_{4-n}	D	$^0\chi$	$^1\chi$	χ_t	D^v	$^0\chi^v$	$^1\chi^v$	χ_t^v
CH_3F	2	2	1	1	8	1.37796	0.37796	0.37796
CH_2F_2	4	2.70711	1.41421	0.70711	16	1.46304	0.53452	0.10102
CHF_3	6	3.57735	1.73205	0.57735	24	1.71124	0.65465	0.03117
CF_4	8	4.5	2	0.5	32	2.01186	0.75593	0.01020
CH_3Cl	2	2	1	1	2	2	1	1
CH_2Cl_2	4	2.70711	1.41421	0.70711	4	2.70711	1.41421	0.70711
$CHCl_3$	6	3.57735	1.73205	0.57735	6	3.57735	1.73205	0.57735
CCl_4	8	4.5	2	0.5	7.12	5.02911	2.26455	0.82183
$CFCl_3$	8	4.5	2	0.5	14	3.87796	1.68898	0.18898
CF_2Cl_2	8	4.5	2	0.5	20	3.25593	1.37796	0.07143
$CHFCl_2$	6	3.57735	1.73205	0.57735	12	2.95531	2.37292	0.21822
CHF_2Cl	6	3.57735	1.73205	0.57735	18	2.33328	1.01379	0.08248
CF_3Cl	8	4.5	2	0.5	26	2.63389	1.06695	0.027
CH_2FCl	4	2.70711	1.41421	0.70711	10	2.08507	0.97437	0.26726
CH_3Br	2	2	1	1	1.33	2.74078	1.74078	1.74078
CH_2Br_2	4	2.70711	1.41421	0.70711	2.52	4.26943	2.77350	2.71964
$CHBr_3$	6	3.57735	1.73205	0.57735	3.99	5.79968	3.01511	3.04557
CBr_4	8	4.5	2	0.5	5.33	7.43953	3.46583	4.52946
CF_3Br	8	4.5	2	0.5	25.33	3.37467	1.43734	0.047
CF_2Br_2	8	4.5	2	0.5	18.66	4.73784	2.11874	0.21645
$CFBr_3$	8	4.5	2	0.5	12.00	6.07672	2.78836	0.98346
CCl_3Br	8	4.5	2	0.5	7.33	5.23292	2.36646	0.86646
CCl_2Br_2	8	4.5	2	0.5	6.67	5.96583	2.73292	1.50150
$CClBr_3$	8	4.5	2	0.5	6.00	6.69875	3.09938	2.60198
CH_2FBr	4	2.70711	1.41121	0.70711	9.33	2.81799	1.49262	0.46314
CH_2ClBr	4	2.70711	1.41121	0.70711	3.33	3.44002	1.93246	1.22536
$CHFClBr$	6	3.57735	1.73205	0.57735	11.33	3.68823	1.79607	0.37815
CHF_2Br	6	3.57735	1.73205	0.57735	17.33	3.06620	1.43694	0.14293
$CHFBr_2$	6	3.57735	1.73205	0.57735	10.66	4.42115	2.21922	0.65931
$CHCl_2Br$	6	3.57735	1.73205	0.57735	5.33	4.31027	2.15520	1.00050
$CHClBr_2$	6	3.57735	1.73205	0.57735	4.66	5.04319	2.57835	1.73378
$CFCl_2Br$	8	4.5	2	0.5	13.33	4.61088	2.05544	0.32749
$CFClBr_2$	8	4.5	2	0.5	12.67	5.34380	2.42190	0.56751
CF_2ClBr	8	4.5	2	0.5	19.33	3.98885	1.74442	0.12378

[a] Here, the algorithm for δ^v depends on the odd-K_p-graph: $\delta^v = \delta^v(ps)/[p \cdot r+1]$: $\delta^v(F) = 7$, $\delta^v(Cl) = 1$, $\delta^v(Br) = 0.33$.

Table 5. Dual and Soft Dual Molecular Connectivity Indices for Halomethanes[a]

CH_nX_{4-n}	$^0\chi_d$	$^1\chi_d$	$^1\chi_s$	$^0\chi^v{}_d$	$^1\chi^v{}_d$	$^1\chi^v{}_s$
CH_3F	0.25	−1	0.70711	1.75	−4	0.35355
CH_2F_2	−0.25	2.25	0.33333	−12.25	20.25	0.11111
CHF_3	0.18750	−8	0.125	64.3125	−125	0.03162
CF_4	−0.125	39.0625	0.04	−300.125	915.063	0.00826
CH_3Cl	0.25	−1	0.70711	0.25	−1	0.70711
CH_2Cl_2	−0.25	2.25	0.33333	−0.25	2.25	0.33333
$CHCl_3$	0.18750	−8	0.125	0.18750	−8	0.125
CCl_4	−0.125	39.0625	0.04	−0.04627	36.6281	0.04377
$CFCl_3$	−0.125	39.0625	0.04	−0.875	85.9375	0.02697
CF_2Cl_2	−0.125	30.0625	0.04	−6.125	189.063	0.01818
$CHFCl_2$	0.18750	−8	0.125	1.31250	−40	0.05590
CHF_2Cl	0.18750	−8	0.125	9.18750	−50	0.05
CF_3Cl	−0.125	39.0625	0.04	−42.875	415.938	0.01296
CH_2FCl	−0.25	2.25	0.33333	−1.75	6.75	0.19245
CH_3Br	0.25	−1	0.70711	0.08250	−0.665	0.86711
CH_2Br_2	−0.25	2.25	0.33333	−0.01690	1.27690	0.44248
$CHBr_3$	0.18750	−8	0.125	0.00674	−4.61575	0.16456
CBr_4	−0.125	30.0625	0.04	−0.00152	22.0310	0.05326
CF_3Br	−0.125	39.0625	0.04	−14.1488	360.202	0.01317
CF_2Br_2	−0.125	39.0625	0.04	−0.66701	141.789	0.021
$CFBr_3$	−0.125	39.0625	0.04	−0.03231	55.9292	0.03343
CCl_3Br	−0.125	39.0625	0.04	−0.04163	33.8516	0.04297
CCl_2Br_2	−0.125	39.0625	0.04	−0.01386	29.3358	0.04616
$CClBr_3$	−0.125	39.0625	0.04	−0.00462	25.4224	0.04958
CH_2FBr	−0.25	2.25	0.33333	−0.58275	5.24925	0.21823
CH_2ClBr	−0.25	2.25	0.33333	−0.08325	1.74975	0.37799
$CHFClBr$	0.18750	−8	0.125	0.43706	−16.665	0.08661
CHF_2Br	0.18750	− 8	0.125	3.05944	−41.6625	0.05478
$CHFBr_2$	0.18750	− 8	0.125	0.14554	−13.8861	0.09488
$CHCl_2Br$	0.18750	− 8	0.125	0.06244	−6.666	0.13694
$CHClBr_2$	0.18750	− 8	0.125	0.02079	−5.55444	0.15002
$CFCl_2Br$	−0.125	30.0625	0.04	−0.29138	74.4734	0.02897
$CFClBr_2$	−0.125	30.0625	0.04	−0.09703	64.5387	0.03112
CF_2ClBr	−0.125	30.0625	0.04	−2.03963	163.8416	0.01953

[a] Here the algorithm for δ^v depends on the odd-K_p-graph (see Table 4, headings).

Table 6. Molecular Pseudoconnectivity Indices for Halomethanes[a]

CH_nX_{4-n}	${}^{S}\psi_I$	${}^{0}\psi_I$	${}^{1}\psi_I$	${}^{T}\psi_I$	${}^{S}\psi_E$	${}^{0}\psi_E$	${}^{1}\psi_E$	${}^{T}\psi_E$
CH_3F	10	1.06066	0.25	0.25	23.22	0.62425	0.09347	0.09347
CH_2F_2	17.50	1.52360	0.57735	0.10206	37.34	0.94990	0.22512	0.02793
CHF_3	25.33	1.92777	0.91971	0.03832	51.84	1.32628	0.43336	0.00886
CF_4	33.25	2.30864	1.27837	0.01398	66.31	1.93991	0.94038	0.00357
CH_3Cl	6.11	1.20037	0.34879	0.34879	19.38	0.64928	0.10465	0.10465
CH_2Cl_2	9.72	1.80302	0.80550	0.19866	29.61	0.97555	0.22699	0.03361
$CHCl_3$	13.66	2.34690	1.28314	0.10407	40.06	1.30162	0.36705	0.01073
CCl_4	17.69	2.86748	1.76475	0.05295	50.60	1.63191	0.52981	0.00344
$CFCl_3$	21.58	2.72777	1.63979	0.03795	54.62	1.64110	0.56935	0.00326
CF_2Cl_2	25.47	2.58794	1.51472	0.0272	58.53	1.66997	0.62811	0.00315
$CHFCl_2$	17.56	2.20609	1.16059	0.07449	44	1.29723	0.38215	0.00994
CHF_2Cl	21.44	2.06644	1.03963	0.05340	47.89	1.30238	0.40275	0.00931
CF_3Cl	29.36	2.44835	1.38987	0.01950	62.41	1.74087	0.72630	0.00318
CH_2FCl	13.61	1.66325	0.69137	0.14238	33.44	0.96129	0.22562	0.03066
CH_3Br	4.75	1.31013	0.42640	0.42640	17.97	0.66822	0.11152	0.11152
CH_2Br_2	7	2.02254	0.98473	0.29691	26.83	1.00855	0.235	0.03779
$CHBr_3$	9.58	2.67618	1.56866	0.19014	36.04	1.34350	0.36685	0.01258
CBr_4	12.25	3.30652	2.15744	0.11827	43.31	1.67844	0.50828	0.00418
CF_3Br	28	2.55811	1.48804	0.02384	61.05	1.72679	0.69680	0.00328
CF_2Br_2	22.75	2.80758	1.71118	0.04066	55.74	1.68061	0.60157	0.00347
$CFBr_3$	17.50	3.05705	1.93431	0.06934	50.56	1.67207	0.54611	0.00378
CCl_3Br	16.33	2.97706	1.86276	0.06471	49.39	1.64222	0.52339	0.0036
CCl_2Br_2	14.97	3.08688	1.96099	0.07912	48.03	1.65445	0.51814	0.00379
$CClBr_3$	13.61	3.19670	2.05921	0.09673	46.67	1.66653	0.51309	0.00398
CH_2FBr	12.25	1.77307	0.78104	0.17408	32.08	0.97800	0.23164	0.03255
CH_2ClBr	8.36	1.91272	0.89507	0.24284	28.19	0.99270	0.23142	0.03571
$CHFClBr$	16.19	2.31591	1.25570	0.09108	48.80	1.25194	0.35625	0.00844
CHF_2Br	20.08	2.17626	1.13475	0.06529	46.53	1.31375	0.40183	0.00983
$CHFBr_2$	14.83	2.42573	1.35082	0.11135	41.28	1.32501	0.38191	0.01111
$CHCl_2Br$	12.31	2.45556	1.37666	0.12705	38.75	1.31555	0.36703	0.01131
$CHClBr_2$	10.94	2.56538	1.47178	0.15534	37.39	1.32980	0.36705	0.01194
$CFCl_2Br$	20.22	2.83741	1.73786	0.04639	53.28	1.65077	0.56091	0.00342
$CFClBr_2$	18.86	2.94723	1.83608	0.05671	51.91	1.66127	0.55323	0.00360
CF_2ClBr	24.11	2.69776	1.61294	0.03325	57.17	1.67333	0.61356	0.00330

[a] ψ_E indices have been rescaled to the S value of Si, $S[Si(SiF_4)] = -6.611$ (see method section).

Table 7. Dual and Soft Dual Molecular Pseudoconnectivity Indices for Halomethenes[a]

CH_nX_{4-n}	${}^{0}\psi_{Id}$	${}^{1}\psi_{Id}$	${}^{1}\psi_{Is}$	${}^{0}\psi_{Ed}$	${}^{1}\psi_{Ed}$	${}^{1}\psi_{Es}$
CH_3F	4	−5	0.31623	28.6178	−11.6050	0.20757
CH_2F_2	−12	22.5625	0.10526	−160.206	111.303	0.04739
CHF_3	42.56	−101.521	0.03509	795.775	−890.277	0.01185
CF_4	−160	452.612	0.01175	−2448.63	5742.16	0.00330
CH_3Cl	2.055	−3.055	0.40456	22.826	−9.69	0.22716
CH_2Cl_2	−3.16727	7.86803	0.17825	−110.628	82.9010	0.05491
$CHCl_3$	5.77108	−20.1237	0.07881	542.615	−642.736	0.01395
CCl_4	−11.1462	51.5869	0.03481	−2639.0	4521.22	0.00372
$CFCl_3$	−21.6958	89.0259	0.02650	−2948.49	4587.89	0.00369
CF_2Cl_2	−42.2508	153.693	0.02017	−3143.72	4744.83	0.00363
$CHFCl_2$	11.2641	−34.5754	0.06013	632.028	−693.901	0.01340
CHF_2Cl	21.9199	−59.2749	0.04592	721.3087	−769.521	0.01275
CF_3Cl	−82.2	265.137	0.01535	−3086.31	5082.97	0.00351
CH_2FCl	−6.16650	13.3261	0.13697	−132.991	94.8608	0.05134
CH_3Br	1.375	−2.375	0.45883	20.1028	- 8.985	0.23590
CH_2Br_2	−1.41797	4.51563	0.23529	−87.5477	73.6164	0.05828
$CHBr_3$	1.72874	−8.48966	0.12134	394.882	−571.787	0.01479
CBr_4	−2.23404	16	0.0625	−1786.07	4196.24	0.00386
CF_3Br	−55	197.86	0.01777	−2906.23	4677.38	0.00366
CF_2Br_2	−18.9063	85.5625	0.02703	−2594.58	4245.73	0.00384
$CFBr_3$	−6.49902	37	0.04110	−2183.30	4134.21	0.00389
CCl_3Br	−7.46337	38.5192	0.04028	−2410.85	4433.85	0.00375
CCl_2Br_2	−4.99253	28.7403	0.04663	−2177.34	4332.47	0.00380
$CClBr_3$	−3.33969	21.4440	0.05399	−1970.21	4254.99	0.00383
CH_2FBr	−4.125	10.0938	0.1574	−117.970	87.7317	0.05338
CH_2ClBr	−2.11973	5.96169	0.20478	−98.0347	77.8062	0.05668
$CHFClBr$	7.53495	−25.9316	0.06943	877.736	−900.986	0.01178
CHF_2Br	14.6630	−44.4562	0.05303	646.645	−713.886	0.01323
$CHFBr_2$	5.04041	−19.4487	0.08017	506.332	−621.694	0.01418
$CHCl_2Br$	3.87202	−15.1261	0.9091	488.187	−616.240	0.01424
$CHClBr_2$	2.59014	−11.3445	0.10497	438.289	−592.120	0.01453
$CFCl_2Br$	−14.5237	66.4620	0.03067	−2668.52	4403.28	0.00377
$CFClBr_2$	−9.71545	49.5893	0.03550	−2412.05	4252.18	0.00383
CF_2ClBr	−28.2631	114.677	0.02335	−2871.96	4471.69	0.00374

[a] ψ_E indices have been rescaled to the S value of Si, $S[Si(SiF_4)] = -6.611$.

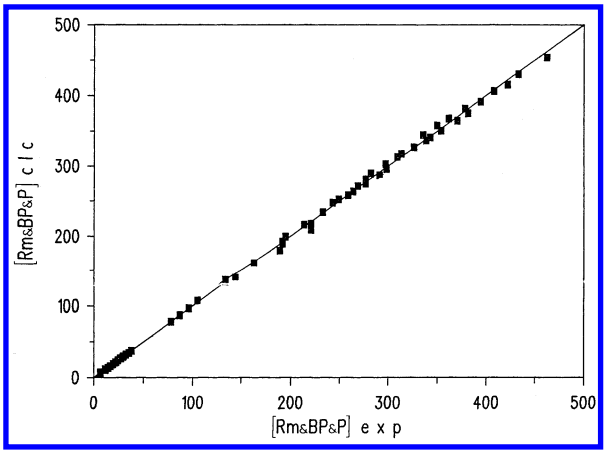

Figure 3. Plot of the calculated R_m, BP, and, $\mathscr{P}$ vs their corresponding experimental values for a total of 77 points.

Here $X = ({}^0\chi^v)^{0.3}$: $Q = 0.136$, $F = 692$, $r = 0.995$, $s_R = 2.06$

$X' = (X - 3\cdot10^{-5.1}\chi^v_d)^{0.8}$: $Q = 0.175$, $F = 1153$, $r = 0.997$, $s_R = 2.66$, $n = 9$, $\mathbf{u} = (34, 23)$, $\langle u \rangle = 29$

Practically, vector $\beta = ({}^S\psi_I, {}^1\psi_I, \chi_t, U_0)$ can be used to model $n = 77$ points. Figure 3, where the experimental R_m, BP, and $\mathscr{P}$ values have been plotted vs their corresponding calculated values, has been obtained with the β vector and with the three correlation vectors for the three properties: $\mathbf{C}(R_m) = (-0.78866, 17.07997, 0, 10.6894)$, $\mathbf{C}(BP) = (-11.3773, 87.2807, -227.493, 519.035)$, and $\mathbf{C}(\mathscr{P}) = (-3.6285, 110.4638, 0, 86.86556)$. Here the correlation coefficient, c_3, for χ_t for R_m and $\mathscr{P}$ is zero.

Dipole Moment, μ. The molar mass is not a good descriptor for the dipole moments of 23 halomethane, as follows: $Q = 1.117$, $F = 13$, $r = 0.618$, $s_R = 0.56$, $n = 23$. Even if a similar deterioration, from R_m to μ is detected for the modeling quality of the connectivity and pseudoconnectivity indices, nevertheless the two-mixed basis index combination shows an interesting modeling quality (note all along this modeling the importance of the zeroth-order basis index)

$\{{}^0\chi\}$: $Q = 2.899$, $F = 87$, $r = 0.898$, $s_0 = 0.31$, $n = 23$, $\mathbf{u} = (8.6, 13)$, $\langle u \rangle = 11$

$\{D^v, {}^1\psi_E\}$: $Q = 5.446$, $F = 154$, $r = 0.969$, $s_R = 1.72$, $n = 23$, $\mathbf{u} = (8.8, 17, 16)$, $\langle u \rangle = 17$

$\mathbf{C} = (-0.057899, -4.39051, 2.18612)$

This property should be modeled with the modulus equation, $\mu = |S\cdot\mathbf{C}|$, where $S = ({}^0\chi, {}^0\psi_I, U_0)$, to avoid a negative dipole moment value for CF_4. Here, the following optimal terms could be found

$X = ({}^0\chi)^{4.5}$, $Q = 3.84$, $F = 154$, $r = 0.938$, $s_R = 1.29$, $n = 23$

$Y = ({}^1\psi_E)\cdot({}^1\psi_I)^{1.4}$, $Q = 4.587$, $F = 219$, $r = 0.955$, $s_R = 1.48$, $n = 23$

$Y' = [Y^{0.8} + 0.5\cdot({}^1\chi^v_s)^{0.3}]$, $Q = 4.992$, $F = 259$, $r = 0.962$, $s_R = 1.63$, $n = 23$, $\mathbf{u} = (16, 39)$, $\langle u \rangle = 28$

Neither a Z- nor a Z′-type term could be detected.

Ionization Potential, IP. The description deteriorates further with this property, where the molar mass shows $Q = 0.35$, $F = 0.9$, $r = 0.274$, $s_R = 0.5$, and $n = 13$. A valence connectivity index and a two-mixed index combination show some descriptive quality

$\{\chi_t^v\}$: $Q = 1.899$, $F = 27$, $r = 0.844$, $s_0 = 0.44$, $n = 13$, $\mathbf{u} = (5.2, 65)$, $\langle u \rangle = 35$

$\{\chi_t^v, {}^T\psi_E\}$: $Q = 2.494$, $F = 23$, $r = 0.908$, $s_R = 1.22$, $n = 13$, $\mathbf{u} = (6.5, 2.5, 79)$, $\langle u \rangle = 29$

A CI-GTBI discovers neither a Y nor a Z term but a very interesting, X′-type term, where term $X = [\chi_t - 1.2\cdot(\chi_t^v)^{0.8}]$ has $Q = 2.543$, $F = 49$, $r = 0.903$, $s_R = 1.24$

$$X' = [X + 0.01\cdot{}^0\chi^v_d]$$

$Q = 3.423$, $F = 88$, $r = 0.943$, $s_R = 1.60$, $n = 13$, $\mathbf{u} = (9.4, 151)$, $\langle u \rangle = 80$

$$\mathbf{C} = (1.70258, 11.8899)$$

Note the importance, for IP, of the total connectivity and pseudoconnectivity indices, i.e., of a type of basis indices that describes the overall chemical graph or pseudograph.

Let us, now, try the second type of valence molecular connectivity basis indices, χ^v, i.e, those basis indices that are shown in Table 8 and that have been calculated with the Z-algorithm.

(2) Z-Algorithm, $\delta^v = Z^v/(Z - Z^v - 1)$, $Z^v = 7$, and Z(F) = 9, Z(Cl) = 17, Z(Br) = 35. *Molar Refraction, R_m.* The best single basis index is, like for the preceding R_m case ($s_0 = 1.71$, see previous section)

$\{{}^0\chi^v\}$: $Q = 0.442$, $F = 463$, $r = 0.967$, $s_R = 0.78$, $n = 34$, $\mathbf{u} = (22, 0.2)$, $\langle u \rangle = 11$

This descriptor cannot compete, at any statistical level, with the preceding best single $\{{}^0\chi^v\}$ descriptor for R_m calculated by the aid of the odd-K_p-graphs. The two-basis-index descriptor is always $\{{}^S\psi_I, {}^1\psi_I\}$, and no higher-order terms with the new χ^v indices could be found.

Boiling Point, BP. The best single basis descriptor is even here, as in the preceding BP case ($s_0 = 29.9$)

$\{{}^1\chi^v\}$: $Q = 0.030$, $F = 183$, $r = 0.923$, $s_R = 0.99$, $n = 34$, $\mathbf{u} = (14, 11)$, $\langle u \rangle = 12$

The descriptive quality is worse than in the preceding BP case, even if the two statistical performances are rather similar. No good two-basis-index combinations and no good terms could be found with these χ^v indices based on a Z-algorithm.

Parachor, $\mathscr{P}$. Here the best single basis descriptor is ${}^1\chi^v$ instead of ${}^0\chi^v$, but its statistical Q/F performance is nearly half of the corresponding odd complete graph case (here, $s_0 = 15.1$)

Table 8. Valence Connectivity Indices for Halomethans[a]

CH_nX_{4-n}	D^v	$^0\chi^v$	$^1\chi^v$	χ_t^v	$^0\chi^v_d$	$^1\chi^v_d$	$^1\chi^v_s$
CH_3F	8	1.37796	0.37796	0.37796	1.75	−4	0.35355
CH_2F_2	16	1.46304	0.53452	0.10102	−12.25	20.25	0.11111
CHF_3	24	1.71124	0.65465	0.03117	64.3125	−125	0.03162
CF_4	32	2.01186	0.75593	0.01020	−300.125	915.063	0.00826
CH_3Cl	1.78	2.13228	1.13228	1.13228	0.195	−0.890	0.74953
CH_2Cl_2	3.56	2.97166	1.60128	0.90655	−0.15210	1.93210	0.35971
$CHCl_3$	5.34	3.97418	1.96116	0.83810	0.08898	−6.75127	0.13607
CCl_4	7.12	5.02911	2.26455	0.82183	−0.04627	36.6281	0.04377
$CFCl_3$	13.34	4.27480	1.88740	0.27433	−0.41523	75.0856	0.02885
CF_2Cl_2	19.56	3.52339	1.51170	0.09181	−3.70736	172.646	0.01903
$CHFCl_2$	11.56	3.22278	1.52734	0.28049	0.79444	−17.8416	0.08370
CHF_2Cl	17.78	2.46701	1.09100	0.09351	7.14787	−47.2250	0.05145
CF_3Cl	25.78	2.76617	1.13309	0.03057	−33.4425	397.636	0.01254
CH_2FCl	9.78	2.21880	1.06893	0.30300	−1.36150	6.25050	0.19999
CH_3Br	1.26	2.96116	1.96116	1.96116	0.065	−0.63	0.89087
CH_2Br_2	2.52	4.26943	2.77350	2.71964	−0.01690	1.27690	0.44248
$CHBr_3$	3.78	6.46083	3.39683	4.35491	0.00330	−4.33075	0.16989
CBr_4	5.04	8.35978	3.92989	7.45367	−0.00056	20.5641	0.05513
CF_3Br	25.26	3.59505	1.54753	0.05295	−11.1475	354.379	0.01328
CF_2Br_2	18.52	5.17825	2.33913	0.27473	−0.41405	137.241	0.02134
$CFBr_3$	11.78	6.77280	3.13640	1.43374	−0.01520	53.1124	0.03430
CCl_3Br	6.59	5.86614	2.68307	1.43170	−0.01525	29.0353	0.04640
CCl_2Br_2	6.07	6.69735	3.09868	2.48136	−0.00508	25.8814	0.04914
$CClBr_3$	5.56	7.52856	3.51428	4.30061	−0.00169	27.0701	0.05205
CH_2FBr	9.26	3.05001	1.65669	0.52515	−0.45325	5.08275	0.22178
CH_2ClBr	3.04	3.80578	2.19109	1.57523	−0.05038	1.56888	0.39919
$CHFClBr$	11.04	4.05399	2.00724	0.48613	0.26447	−15.3906	0.09012
CHF_2Br	17.26	3.29822	1.57090	0.16207	2.37956	−40.7375	0.05539
$CHFBr_2$	10.52	4.88520	2.48714	0.84254	0.08804	−13.2764	0.09703
$CHCl_2Br$	4.81	4.82124	2.44358	1.46669	0.02905	−5.81458	0.14662
$CHClBr_2$	4.30	5.64097	2.92348	2.52726	0.00979	−5.01581	0.15786
$CFCl_2Br$	12.82	5.11037	2.30519	0.47730	−0.13717	66.8456	0.03058
$CFClBr_2$	12.30	5.94158	2.72079	0.82724	−0.04567	59.5846	0.03239
CF_2ClBr	10.04	4.35460	1.92730	0.15912	−1.23420	153.893	0.02015

[a] The δ^valgorithm is $\delta^v = Z^v/(Z-Z^v-1)$, $\delta^v(F) = 7$, $\delta^v(Cl) = 0.78$, $\delta^v(Br) = 0.26$.

$\{^1\chi^v\}$: Q = 0.046, F = 80, r = 0.959, s_R = 0.73, n = 9, **u** = (8.9, 5.1), ⟨*u*⟩ = 7

No better or even similar CI-GTBI of any kind could be detected.

Dipole Moment, μ. Here, neither the $^0\chi^v$ best index (instead of $^0\chi$) nor combinations of basis indices or even higher-order terms could compete, by far, with the preceding descriptors for μ. For sheer curiosity the statistics of the best index, $\{^0\chi^v\}$, are as follows: Q = 1.257, F = 16, r = 0.662, s_R = 0.58, n = 23 (s_0 = 0.31).

Ionization Potential, IP. This is the only property where the Z-algorithm based χ^v indices show interesting results. In fact, we have the following better, single- and two-basis-index descriptions, and X-type term (s_0 = 0.44)

$\{\chi_t^v\}$: Q = 2.621, F = 52, r = 0.908, s_R = 1.26, n = 13, **u** = (7.2, 79), ⟨u⟩ = 44

$\{\chi_t^v, ^T\psi_E\}$: Q = 2.959, F = 33, r = 0.932, s_R = 1.42, n = 13, **u** = (5.8, 1.8, 87), ⟨u⟩ = 31

$X = (\chi_t - 1.2\cdot\chi_t^v)$: Q = 3.136, F = 74, r = 0.933, s_R = 1.48, n = 13, **u** = (8.6, 135), ⟨u⟩ = 72

No optimal X′-type term could be found (see preceding case). Note that the type of basis indices does not change, i.e., ionization energies are only modeled by the total type of basis indices, χ_t, χ_t^v, and $^T\psi_E$. The end result is that the best description for this property continues to be the preceding one, with the X′ term based on valence indices obtained with the odd complete graph algorithm.

(3) Homogeneous-Algorithm, $\delta^v = (2/n)^2\delta^v$(ps): n(F) = 2, n(Cl) = 3, and n(Br) = 4, and δ^v(ps) = 7. *Molar Refraction, R_m.* Comparison with the two preceding cases shows that this is the worst description, in fact, the best single basis descriptor, $\{^1\chi^v\}$, shows

$\{^1\chi^v\}$: Q = 0.382, F = 345, r = 0.957, s_R = 0.19, n = 34, **u** = (19, 6.2), ⟨u⟩ = 12

The only interesting characteristic, here, being c_o value improves (6.2 instead of 0.2). The s_0 values used all along this section are taken from the first section, here s_0 = 1.71. This homogeneous-algorithm case, nevertheless, shows a rather good two-basis-index description, whose statistical values are not that far from the statistical values of the odd complete graph case

$\{D^v, ^1\psi_I\}$: Q = 4.181, F = 20681, r = 0.996, s_R = 7.13, n = 34, **u** = (123, 196, 72), ⟨u⟩ = 130

Better descriptions could not be found with any type of term.

Boiling Point, BP. The best single basis descriptor is here, like in the two preceding BP cases, $^1\chi^v$, but here the quality of the description is deceiving (here, s_0 = 29.9)

$\{^1\chi^v\}$: Q = 0.021, F = 84, r = 0.851, s_R = 0.72, n = 34, **u** = (14, 11), ⟨u⟩ = 12

Instead, a quite satisfactory two-basis-index descriptor could be found

$\{^0\chi, D^v\}$: Q = 0.108, F = 1155, r = 0.993, s_R = 3.25, n = 34, **u** = (41, 47, 3.2), ⟨u⟩ = 30

The only statistical value that differs consistently from the odd complete graph case is the c_0 value (3.2 instead of 6.6). Like in the two preceding BP cases no improved CI-GTBI could be detected.

Parachor, $\mathscr{P}$. The best single basis descriptor is again $^0\chi^v$, like in the odd complete graph case. Its statistics are much better than the statistics of the Z-algorithm case and a bit better than the statistics of the odd complete graph case, but with a useless c_o = 0.8 value (here, s_0 = 15.1)

$\{^0\chi^v\}$: Q = 0.069, F = 178, r = 0.981, s_R = 1.06, n = 9, **u** = (13, 0.8), ⟨u⟩ = 7.1

This negative feature is corrected by the two-basis-index descriptor, whose statistics are nevertheless not better than the statistics of the odd complete graph case

$\{D^v, {}^1\psi_I\}$: Q = 0.383, F = 2750, r = 0.9995, s_R = 5.79, n = 9, **u** = (30, 72, 27), ⟨u⟩ = 43

An interesting X′-type CI-GTBI could be detected, where $X = (^0\chi^v)^{1.4}$: Q = 0.074, F = 204, r = 0.983, and s_R = 1.13. Its statistics are, nevertheless, not better than in the K_p case

$X' = (X - 6\cdot10^{-4.1}\chi^v_d)$: Q = 0.111, F = 462, r = 0.993, s_R = 1.69, n = 9, **u** = (21, 8.5), ⟨u⟩ = 15

Dipole Moment, μ. Comparison with the preceding Z-algorithm case shows that here the modeling improves but not enough to compete with the modeling achieved by the odd complete graph case. Index $^0\chi^v$ is, even here, the best single descriptor with the following: Q = 1.257, F = 16, r = 0.662, s_R = 0.58, n = 23 (s_0 = 0.31). This is a rather poor description, indeed. The best two-basis-index combination is as follows: $\{D^v,{}^1\psi_E\}$, a combination already detected along the odd complete graph case, but not as good

$\{D^v, {}^1\psi_E\}$: Q = 4.105, F = 88, r = 0.947, s_R = 1.35, n = 23, **u** = (6.1, 11, 18), ⟨u⟩ = 12

Also here an interesting, but not as good, X term could be detected, and this is the only kind of term that can be detected

$X = (^0\chi^v)^{0.01}$, Q = 2.029, F = 43, r = 0.819, s_R = 0.78, **u** = (6.5, 6.6) ⟨u⟩ = 6.6

Ionization Potential, IP. The χ^v indices based on the homogeneous algorithm shows a deterioration of the modeling quality relative to the Z-algorithm, in fact (s_0 = 0.44)

$\{\chi_t^v\}$: Q = 0.709, F = 3.8, r = 0.506, s_R = 0.62, n = 13

$\{\chi_t^v, {}^T\psi_E\}$: Q = 1.887, F = 13, r = 0.853, s_R = 0.98, n = 13, **u** = (4.8, 4.2, 70), ⟨u⟩ = 26

$X' = [X+0.0004\cdot{}^0\chi^v_d]$: Q = 2.528, F = 48, r = 0.902, s_R = 1.22, n = 13, **u** = (6.9, 21), ⟨u⟩ = 14

Here, $X = [\chi_t - (\chi_t^v)^{0.6}]$: Q = 2.282, F = 39, r = 0.883, s_R = 1.13. Only the X′ term can positively compare with the preceding X(Z)-term but not with the corresponding term of the odd complete graph case. Noteworthy, is the detected regularity shown all along the three IP cases based on the importance of the total type basis indices, χ_t, χ_t^v, and $^T\psi_E$.

There are some other regularities, concerning R_m, BP, $\mathscr{P}$, and μ. For R_m, along the best descriptions (K_p and Z algorithm), the best single index is $^0\chi^v$, for BP, the best single descriptor is, in any case, $^1\chi^v$, for $\mathscr{P}$the best descriptor along the best cases (K_p and homogeneous case) is $^0\chi^v$, and for μ, along the K_p, and homogeneous case, the best descriptor is $\{D^v,{}^1\psi_E\}$.

The Chlorofluorocarbons (CFCs) and the K_p-Odd-Complete-Graph Algorithm. The rates of hydrogen abstraction, logK, that measures the effect of the reactions with the hydroxyl radical and the minimum anesthetic concentration (MAC) measured in units of logMAC of a series of chlorofluorocarbons (CFC) have been studied in the recent past with χ^v-Z-algorithm indices and with pseudobasis indices based on the $(2/n)^2\delta^v$(ps) algorithm.[10,14] Here, the attention will be centered on χ^v based on the odd complete graph conjecture. The property values are collected in Table 10, and the different K_p connectivity and pseudoconnectivity indices are collected in Tables 11 and 12. For comparison purposes (the previous studies did not consider the dual indices[14]) we will here center our attention on the odd complete graph conjecture only. As we shall see, the choice of these two properties of CFCs will also uncover an interesting property of the CI-GTBI.

Rates of Hydrogen Abstraction, logK. The previous modeling of this property performed with connectivity indices which were based on the Z-algorithm gave rise to a satisfactory modeling only at the level of the following CI-GTBI[14]

$$Y = [(^S\psi_E - 1.1\,^S\psi_I - {}^T\psi_I)/{}^0\psi_I]^{6.5}$$

Q = 2.07, F = 63, r = 0.852, s_0 = 0.41, n = 26, ⟨u⟩ = 24, u = (8.0, 41)

$$X = (\chi_t)^4[D^v + 3.5\cdot(^0\chi^v)^{1.2} + 5.8\cdot(\chi_t^v)^{0.4} - 5.2\cdot(^0\chi)]^{4.3}$$

Q = 3.05, F = 137, r = 0.923, s_R = 1.37, n = 26, ⟨u⟩ = 38, **u** = (12, 65)

$$Z = (X)^{0.5}\cdot(Y)^{0.3}$$

Q = 3.41, F = 172, r = 0.937, s_R = 1.52, n = 26, ⟨u⟩ = 33, **u** = (10, 56)

The best X(K_p) term, which is here the only satisfactory K_p descriptor, is the following one that resembles strikingly the preceding X descriptor based on the Z-algorithm but which is not as good

Table 9: Valence Connectivity Indices for Halomethenes[a]

CH_nX_{4-n}	D^v	$^0\chi^v$	$^1\chi^v$	χ_t^v	$^0\chi^v_d$	$^1\chi^v_d$	$^1\chi^v_s$
CH_3F	8	1.37796	0.37796	0.37796	1.75	−4	0.35355
CH_2F_2	16	1.46304	0.53452	0.10102	−12.25	20.25	0.11111
CHF_3	24	1.71124	0.65465	0.03117	64.3125	−125	0.03162
CF_4	32	2.01186	0.75593	0.01020	−300.125	915.063	0.00826
CH_3Cl	4.11	1.56705	0.56705	0.56705	0.77750	−2.0055	0.49326
CH_2Cl_2	8.22	1.84120	0.80193	0.22737	−2.41802	6.52802	0.19569
$CHCl_3$	12.33	2.27849	0.98216	0.10527	5.64004	−28.5124	0.06621
CCl_4	16.44	2.76819	1.13410	0.05170	−11.6937	159.720	0.01978
$CFCl_3$	20.33	2.57911	1.03955	0.03446	−26.3202	247.105	0.01590
CF_2Cl_2	24.22	2.38984	0.94492	0.02296	−59.2797	382.408	0.01278
$CHFCl_2$	16.22	2.08923	0.87288	0.07014	12.7028	−46.6804	0.05175
CHF_2Cl	20.11	1.90024	0.76377	0.04676	28.5823	−76.3875	0.04045
CF_3Cl	28.11	2.20094	0.85047	0.01531	−133.341	591.453	0.01028
CH_2FCl	12.11	1.65203	0.66816	0.15153	−5.44425	11.4998	0.14744
CH_3Br	2.75	1.75593	0.75593	0.75593	0.43750	−1.375	0.60302
CH_2Br_2	5.5	2.21896	1.06904	0.40406	−0.76563	3.51563	0.26667
$CHBr_3$	8.25	2.84514	1.30931	0.24939	1.00488	−13.3965	0.09660
CBr_4	11.00	3.52372	1.51186	0.16327	−1.17236	68.3206	0.03025
CF_3Br	26.75	2.38982	0.94491	0.02041	−75.0313	478.328	0.01143
CF_2Br_2	21.50	2.76779	1.13389	0.04082	−18.7478	250.035	0.01581
$CFBr_3$	16.25	3.14575	1.32288	0.08163	−4.68945	130.700	0.02187
CCl_3Br	15.08	2.95680	1.22840	0.06888	−6.58640	129.223	0.02299
CCl_2Br_2	13.72	3.14577	1.32289	0.09184	−3.70498	104.491	0.02446
$CClBr_3$	12.36	3.33474	1.41737	0.12245	−2.08413	84.4917	0.02720
CH_2FBr	10.75	1.84100	0.80178	0.20203	−3.06250	8.43750	0.17213
CH_2ClBr	6.86	2.02999	0.93542	0.30305	−1.36106	4.79156	0.22842
$CHFClBr$	14.86	1.27820	0.98199	0.09352	7.14558	−36.2841	0.05870
CHF_2Br	18.75	2.08921	0.87287	0.06235	16.0781	−59.3750	0.04588
$CHFBr_2$	13.50	2.46717	1.09109	0.12470	4.01953	−28.2031	0.06657
$CHCl_2Br$	10.97	2.46719	1.09110	0.14029	3.17570	−22.1732	0.07508
$CHClBr_2$	9.61	2.65617	1.20020	0.18705	1.78639	−17.2349	0.08516
$CFCl_2Br$	18.97	2.76781	1.13390	0.04592	−14.8199	199.895	0.01768
$CFClBr_2$	17.61	2.95678	1.22839	0.06123	−8.33651	161.636	0.01966
CF_2ClBr	22.86	2.57881	1.03941	0.03061	−33.3460	309.217	0.01422

[a] The δ^valgorithm is $\delta^v = (2/n)^2\delta^v(ps)$, $\delta^v(F) = 7$, $\delta^v(Cl) = 3.11$, $\delta^v(Br) = 1.75$.

$$X(K_p) = (\chi_t)^{3.9}[D^v + 3.7\cdot(^0\chi^v)^{1.2} + 5.9\cdot(\chi_t v)^{0.5} - 4.2\cdot(^0\chi)]^{4.2}$$

$Q = 2.65$, $F = 104$, $r = 0.901$, $s_R = 1.21$, $n = 26$, $\langle u \rangle = 38$, $\mathbf{u} = (12, 65)$

When this $X(K_p)$ term is used together with the previous Y term to build a mixed higher-order Z_p-type term, two types of Z_p terms can be detected. The first one is very similar to the previous one, while the second one shows the best overall modeling power. No such type of term could be detected with the molecular connectivity indices based on the Z-algorithm.

$$Z_p = [X(K_p)]^{0.5}\cdot(Y)^{0.3}$$

$Q = 3.42$, $F = 173$, $r = 0.937$, $s_R = 1.52$, $n = 26$, $\langle u \rangle = 35$, $\mathbf{u} = (13, 58)$, $\mathbf{C} = (-0.00032, 9.23310)$

$$Z_p = [(X(K_p))^{0.5}\cdot(Y)^{0.3} - (D^v)^{1.9}]^{0.9}$$

$Q = 3.64$, $F = 196$, $r = 0.944$, $s_R = 1.58$, $n = 26$, $\langle u \rangle = 34$, $\mathbf{u} = (14, 54)$, $\mathbf{C} = (-0.00093, 9.57433)$

The Minimum Anesthetic Concentration, logMAC. The previous best descriptors based on $\chi^v = f[Z^v/(Z-Z^v-1)]$ are[14]

$\{^1\chi^v\}$: $Q = 6.65$, $F = 200$, $r = 0.978$, $s_0 = 0.15$, $n = 11$, $\langle u \rangle = 16$, $\mathbf{u} = (14, 17)$

$$Z = [(X)^{0.01} + (Y)^{0.9}]^5$$

$Q = 17.7$, $F = 1414$, $r = 0.997$, $s_R = 2.50$, $n = 11$, $\langle u \rangle = 38$, $\mathbf{u} = (38, 39)$

where $X = (^1\chi^v + 1.2\cdot\chi_t)^{0.5}$: $Q = 7.84$, $F = 278$, $r = 0.981$, and $Y = (^1\psi_I + {}^T\psi_I)/{}^S\psi_E$: $Q = 15.3$, $F = 1065$, $r = 0.996$. The $\chi^v = f(K_p)$ indices instead do not to achieve the same optimal modeling, in fact

$\{^1\chi^v\}$: $Q = 4.87$, $F = 106$, $r = 0.961$, $s_R = 0.75$, $n = 11$, $\langle u \rangle = 12$, $\mathbf{u} = (10, 13)$

$$Z = [(X(K_p))^{0.01} + (Y)^{0.9}]^5$$

$Q = 16.1$, $F = 1165$, $r = 0.996$, $s_R = 2.42$, $n = 11$, $\langle u \rangle = 34$, $\mathbf{u} = (34, 35)$

where $X(K_p) = (0.9\cdot^1\chi^v + \chi_t)^{0.05}$, $Q = 5.43$, $F = 133$, $r = 0.968$, and the Y term is the same of the previous case. But, now, it is possible to detect the following very interesting Z_p term which is formally equal to a very good descriptor found for logK

$$Z_p = [X(K_p)]^{0.5}\cdot(Y)^{0.3}$$

$Q = 18.0$, $F = 1460$, $r = 0.997$, $s_R = 2.73$, $n = 11$, $\langle u \rangle = 39$, $\mathbf{u} = (38, 39)$, $\mathbf{C} = (-52.5598, 20.0485)$

Figure 4 has been obtained with this Z_p term using once the correlation vector for logMAC and the other time the

Table 10. Rates of Hydrogen Abstraction for $n = 26$ CFCs, logK, Logarithm of the Minimum Anesthetic Concentrations, logMAC, for $n = 11$ Trifluoromethyl Ethanes, Each Followed by Calculated P_{clc}, and by the Percent Residual, $\Delta\% = |(p_{ex} - p_{calc})\cdot 100/p_{ex}|$

CFC	logK	P_{clc}	Δ%	CFC	LogMAC	P_{clc}	Δ%
CH_3Cl	7.36	7.65	3.9	CH_2ClCF_3	0.90	0.90	0.001
CH_2Cl_2	8.00	7.98	0.2	$CHCl_2CF_3$	0.43	0.41	0.05
$CHCl_3$	7.80	7.71	1.2	$CHClFCF_3$	1.18	1.12	0.05
CH_3F	6.95	6.98	0.4	CHF_2CF_3	1.70	1.73	0.02
CH_2F_2	6.81	6.60	3.1	CH_3CF_3	1.60	1.63	0.02
CHF_3	5.10	5.39	5.7	CH_2BrCF_3	0.45	0.38	0.2
CH_2ClF	7.46	7.54	1.1	CH_2ICF_3	0.10	0.07	0.3
$CHCl_2F$	7.30	7.39	1.2	$CHFBrCF_3$	0.70	0.66	0.06
$CHClF_2$	6.45	6.62	2.6	$CHFICF_3$	0.30	0.36	0.2
CH_3CH_2Cl	8.37	8.19	2.2	$CHClBrCF_3$	−0.10	−0.0003	1.0
CH_3CH_2F	8.14	7.87	3.3	$CHBr_2CF_3$	−0.40	−0.41	0.02
CH_3CHCl_2	8.20	7.93	3.3				
CH_3CHF_2	7.48	7.04	5.9				
CH_2FCH_2F	7.83	7.71	1.5				
$CH_2ClCHCl_2$	8.28	8.24	0.5				
CH_2FCHF_2	7.47	7.15	4.3				
CH_2ClCF_2Cl	7.20	7.60	5.7				
CH_2ClCF_3	6.95	7.01	0.9				
CH_2FCF_3	6.70	6.36	5.1				
CHF_2CHF_2	6.50	6.72	3.3				
$CHCl_2CF_3$	7.40	7.23	2.3				
$CHClFCF_3$	6.87	6.66	3.0				
CHF_2CF_3	6.48	6.13	5.4				
CH_3CCl_3	6.80	7.51	11				
CH_3CF_3	5.95	5.82	2.2				
CH_3CF_2Cl	6.60	6.69	1.3				

Table 11. Molecular Connectivity χ Values for 32 CFCs[a]

CFC	D	$^0\chi$	$^1\chi$	χ_t	D^v	$^0\chi^v$	$^1\chi^v$	χ_t^v
CH_3Cl	2	2	1	1	2	2	1	1
CH_3F	2	2	1	1	8	1.37796	0.37796	0.37796
CH_2Cl_2	4	2.70711	1.41421	0.70711	4	2.70711	1.41421	0.70711
CH_2F_2	4	2.70711	1.41421	0.70711	16	1.46304	0.53452	0.10102
CH_2ClF	4	2.70711	1.41421	0.70711	10	2.08507	0.97437	0.26726
CH_3CH_2F	4	2.70711	1.41421	0.70711	10	2.08507	0.97437	0.26726
CH_3CH_2Cl	4	2.70711	1.41421	0.70711	4	2.70711	1.41421	0.70711
CHF_3	6	3.57735	1.73205	0.57735	24	1.71124	0.65465	0.03117
$CHCl_2F$	6	3.57735	1.73205	0.57735	12	2.95531	2.37292	0.21822
$CHClF_2$	6	3.57735	1.73205	0.57735	18	2.33328	1.01379	0.08248
$CHCl_3$	6	3.57735	1.73205	0.57735	6	3.57735	1.73205	0.57735
CH_3CHCl_2	6	3.57735	1.73205	0.57735	6	3.57735	1.73205	0.57735
CH_3CHF_2	6	3.57735	1.73205	0.57735	18	2.33328	1.01379	0.08248
CH_2FCH_2F	6	3.41421	1.91421	0.5	18	2.17014	1.03452	0.07143
$CH_2ClCHCl_2$	8	4.28446	2.27006	0.40825	8	4.28446	2.27006	0.40825
CH_2FCHF_2	8	4.28446	2.27006	0.40825	26	2.41835	1.11195	0.02204
CH_2ClCF_2Cl	10	5.20711	2.56066	0.35355	22	3.96304	1.93862	0.5051
CH_2ClCF_3	10	5.20711	2.56066	0.35355	28	3.34100	1.62761	0.01909
CH_2BrCF_3	10	5.20711	2.56066	0.35355	27.33	4.07392	2.14586	0.03308
CH_2ICF_3	10	5.20711	2.56066	0.35355	27.16	4.81789	2.67192	0.04728
CH_3FCF_3	10	5.20711	2.56066	0.35355	34	2.71896	1.18776	0.00722
CHF_2CHF_2	10	5.15470	2.64273	0.33333	34	2.66656	1.20620	0.00680
$CHCl_2CF_3$	12	6.07735	2.94338	0.28868	30	4.21124	2.01032	0.01559
$CHClFCF_3$	12	6.07735	2.94338	0.28868	36	3.58921	1.65119	0.00589
CHF_2CF_3	12	6.07735	2.94338	0.28868	42	2.96717	1.29206	0.00223
$CHClBrCF_3$	12	6.07735	2.94338	0.28868	29.33	4.94416	2.43347	0.02701
$CHFBrCF_3$	12	6.07735	2.94338	0.28868	35.33	4.32213	2.07434	0.1021
$CHFICF_3$	12	6.07735	2.94338	0.28868	35.16	5.06610	2.50387	0.01459
$CHBr_2CF_3$	12	6.07735	2.94338	0.28868	28.67	5.67708	2.85662	0.04681
CH_3CF_3	8	4.5	2	0.5	26.0	2.63389	1.06695	0.02700
CH_3CF_2Cl	8	4.5	2	0.5	20	3.25593	1.37796	0.07143
CH_3CCl_3	8	4.5	2	0.5	8	4.5	2	0.5

[a] Here, the algorithm for δ^v is obtained with the odd complete graph algorithm: $\delta^v = \delta^v(ps)/[p\cdot r+1]$: $\delta^v(F) = 7$, $\delta^v(Cl) = 1$, $\delta^v(Br) = 0.33$.

correlation vector for logK. The calculated values for logMAC and logK (P_{clc}) and the corresponding percent residuals of Table 10 have also been obtained in this way. The leave-one-out values (not shown) show similar results that compare positively with the previous values.[14]

CONCLUSION

The modeling of different properties of different classes of compounds to check the computational advantages of using odd complete graphs for the inner-core electrons shows positive and interesting results. The odd complete graph

Table 12. Molecular Pseudoconnectivity Index Values for $n = 32$ CFCs[a]

CFC[a]	${}^{S}\psi_I$	${}^{0}\psi_I$	${}^{1}\psi_I$	${}^{T}\psi_I$	${}^{S}\psi_E$	${}^{0}\psi_E$	${}^{1}\psi_E$	${}^{T}\psi_E$
CH_3Cl	6.11	1.20037	0.34879	0.34879	17.11	0.69281	0.11895	0.11895
CH_2Cl_2	9.72	1.80302	0.80550	0.19866	26.03	1.04637	0.26291	0.04122
CHCl3	13.66	2.34690	1.28314	0.10407	35.68	1.39314	0.42869	0.01386
CH_3F	10.00	1.06066	0.25000	0.25000	21.00	0.66645	0.10541	0.10541
CH_2F_2	17.50	1.52360	0.57735	0.10206	34.01	1.03057	0.26552	0.03413
CHF_3	25.33	1.92777	0.91971	0.03832	47.34	1.50947	0.56938	0.01251
CH_2ClF	23.61	1.66331	0.69142	0.14239	30.11	1.03275	0.26350	0.03722
$CHCl_2F$	17.55	2.20719	1.16200	0.07559	39.35	1.40229	0.45671	0.01310
$CHClF_2$	21.44	2.06748	1.04085	0.05346	43.45	1.42839	0.49624	0.01245
CH_3CH_2Cl	7.61	2.01687	0.98010	0.28479	24.11	1.07743	0.27124	0.04552
CH_3CH_2F	11.50	1.87716	0.86603	0.20412	28.00	1.06714	0.27526	0.04163
CH_3CHCl_2	11.55	2.56074	1.46857	0.14918	33.56	1.42391	0.43028	0.01539
CH_3CHF_2	19.33	2.28132	1.22628	0.07664	41.32	1.44814	0.49327	0.01376
CH_2FCH_2F	19.00	2.34010	1.24402	0.08333	41.00	1.42984	0.44802	0.01357
$CH_2ClCHCl_2$	15.16	3.16340	1.96617	0.08497	42.67	1.77999	0.58378	0.00534
CH_2FCHF_2	26.83	2.74427	1.60981	0.03129	54.25	1.87126	0.74484	0.00489
CH_2ClCF_2Cl	23.97	3.86045	2.20669	0.04274	59.48	2.25853	0.99310	0.00191
CH_2ClCF_3	30.86	3.26485	2.08173	0.01592	63.85	2.42448	1.23127	0.00208
CH_2FCF_3	34.75	3.12514	1.96766	0.01141	67.74	2.62825	1.53805	0.00235
CHF_2CHF_2	34.66	3.14843	1.97816	0.01175	67.68	2.41002	1.20063	0.00196
$CHCl_2CF_3$	34.80	3.80872	2.57968	0.00834	73.28	2.91742	1.63042	0.00083
$CHClFCF_3$	38.69	3.66901	2.45853	0.00598	77.79	3.26865	2.19995	0.00104
CHF_2CF_3	42.58	3.52930	2.33739	0.00428	81.10	4.55532	4.38982	0.00210
CH_3CCl_3	15.58	3.08133	1.95602	0.07590	43.08	1.77734	0.61915	0.00525
CH_3CF_3	27.25	2.66219	1.58114	0.02795	54.74	1.98926	0.95756	0.00542
CH_3CF_2Cl	23.36	2.80190	1.70610	0.03900	50.78	1.85862	0.77775	0.00509
CH_2BrCF_3	29.50	3.37461	2.17315	0.01941	62.14	2.52461	1.32327	0.00245
CH_2ICF_3	28.87	3.45839	2.39975	0.02217	61.88	2.39562	1.14897	0.00217
$CHFBrCF_3$	37.33	3.77877	2.55371	0.00731	75.84	3.13653	1.95688	0.00100
$CHFICF_3$	36.70	3.86255	2.62635	0.00832	75.22	3.09680	1.87379	0.00100
$CHClBrCF_3$	33.44	3.91848	2.67485	0.01020	71.95	2.86487	1.52435	0.00083
$CHBr_2CF_3$	32.08	4.02824	2.77002	0.01246	70.57	2.82553	1.43874	0.00083

[a] ψ_E values have been obtained with a rescaling procedure ($S[C(CF_4)] = -5.5$, see Method section).

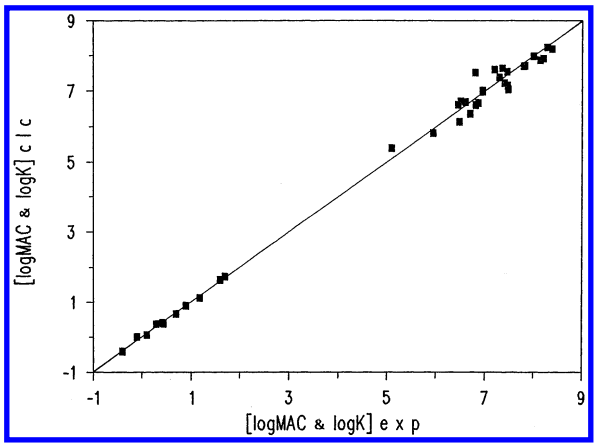

Figure 4. Plot of the calculated vs the experimental logMAC (bottom, left-side) plus logK (top, right-side).

conjecture, when fails at the level of the single basis indices, or its combinations, seems, nevertheless, to work advantageously at the level of the CI-GTBI, which seems to prefer the K_p-odd-complete-graph valence molecular connectivity indices. The homogeneous description based on the $(2/n)^2\delta^v$-(ps) algorithm for χ^v and ψ indices shows, instead, poor results. In addition to the computational advantage offered by this conjecture, there is a theoretical advantage for the introduction of odd complete graphs, as it gives to the whole theory of molecular connectivity a more coherent character. The K_p conjecture for the inner-core electrons has the advantage to render the molecule, together with the pseudograph and graph concept, a pure "graph object", as, now, the entire molecular framework can be "graphically" encoded and used for predictive computations. Clearly this finding is only inductive and has only a heuristic value that should be checked further. In fact, other calculations are underway, to detect new applications of the conjecture, i.e., when and how it works.

At the margin of this conjecture there are other significant results of this study: (i) the importance of the ${}^0\chi^v$ indices, that are atom-based basis indices, in modeling the lattice enthalpies of metal halides, the molar refraction, and the parachor of halomethane, (ii) the importance of the total basis indices and pseudoindices in modeling the ionization potential of halomethane, (iii) the importance of the pseudo basis indices, ψ, in the modeling of R_m, BP, $\mathscr{P}$, and finally (iv) the interesting contribution of the dual indices in enhancing the descriptive quality of some terms.

The idea of a graph representation of a molecule is surely older than a century, the seminal studies of Harry Wiener are more than half a century old,[29] while molecular connectivity is just a bit older than a quarter of a century.[2,5,9] However the creativity they have engendered suggests the words of Bohren and Craig on another topic "*be prepared for a journey, but do not expect a destination*".[30]

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