Wiener Index Extension by Counting Even/Odd Graph Distances

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Chemical structures of organic compounds are characterized numerically by a variety of structural descriptors, one of the earliest and most widely used being the Wiener index *W*, derived from the interatomic distances in a molecular graph. Extensive use of such structural descriptors or topological indices has been made in drug design, screening of chemical databases, and similarity and diversity assessment. A new set of topological indices is introduced representing a partitioning of the Wiener index based on counts of even and odd molecular graph distances. These new indices are further generalized by weighting exponents which can be optimized during the quantitative structure−activity/−property relationship (QSAR/QSPR) modeling process. These novel topological indices are tested in QSPR models for the boiling temperature, molar heat capacity, standard Gibbs energy of formation, vaporization enthalpy, refractive index, and density of alkanes. In many cases, the even/odd distance indices proposed here give notably improved correlations.

INTRODUCTION

The continuous development of structural descriptors and statistical equations transformed quantitative structure−property relationships (QSPR) and quantitative structure−activity relationships (QSAR) into powerful and widely used models for the prediction of physical, chemical, and biological properties.[1−5] During the past 20 years QSPR and QSAR techniques have gained wide acceptance in physical, organic, analytical, pharmaceutical, and medicinal chemistry, biochemistry, chemical engineering and technology, toxicology, and environmental sciences. The success of the QSPR and QSAR approach can be explained by the possibility of estimating the properties of new chemical compounds without the need to synthesize and test them. The main hypothesis in the QSPR and QSAR approach is that all properties (physical, chemical, and biological) of a chemical substance are statistically related to its molecular structure. The chemical structure of organic compounds is represented in a numerical form by various theoretical descriptors; these descriptors are used in a statistical model for the computation of the desired molecular property. An inspection of the published QSPR and QSAR models shows that molecular graph descriptors and topological indices (TIs) are used with success in modeling various properties and demonstrates that they are valuable descriptors of chemical structure.[1−15] Comparative QSPR studies of existing graph descriptors[16−19] clearly indicate that each property is best modeled by a specific descriptor or group of descriptors and that there is enough room for novel descriptors, designed to improve the correlational abilities of present-day topological indices. Another direction of intense research is represented by the parametrization of vertex- and edge-weighted molecular graphs, representing organic compounds with heteroatoms and multiple bonds;[11,20−23] this research direction is stimulated by the novel application of molecular graph descriptors in similarity and diversity assessment, in database mining, and in the virtual screening of combinatorial libraries.[24]

The use of modern TIs in chemistry begins with the Wiener index *W*, which was applied for establishing correlations between molecular structure and physical properties of alkanes.[25] Hosoya extended the original definition to cyclic compounds with the aid of the distance matrix and gave a graph-theoretical formula for the Wiener index as "the half sum of the off-diagonal elements of a distance matrix D whose element d_{ij} is a number of bonds for the shortest path between atoms *i* and *j*".[26] Together with the connectivity indices,[1,2] the Wiener index is the most frequently used graph descriptor in QSAR/QSPR models. Its success stimulated the research in the domain of descriptors based on graph distances, novel molecular matrices,[12] and Wiener-like indices.[13] Elements of the distance matrix were used to define degree−distance VTI indices;[27] such vector−matrix invariants can generate TIs with a low degeneracy. The idea to use reciprocal distances in computing VTI indices was adopted in the definition of the reciprocal distance matrix **RD**.[28−31] Another distance measure was defined as the resistance distance matrix **Ω**;[32] this metric is identical with that induced by the distance matrix only for acyclic compounds, while for cyclic compounds the resistance distance matrix offers the possibility of computing an index related but not identical to the Wiener index. Other recently defined distance-related matrices are the detour **Δ**,[33] detour−distance **Δ**−**D**,[33] distance−valency **Dval**,[34] and complementary distance **CD**[35] matrices. Graph distances were used to define the Wiener polynomial,[36,37] which is the source of novel topological indices used with success in several QSPR models.[38] For bipartite molecular graphs, in which vertices can be separated into starred and unstarred, the Wiener

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number can be separated into three components, representing the distance sums for the three types of pairs of vertices: starred−starred, unstarred−unstarred, and starred−unstarred.[39] Using this separation, it was demonstrated that the degeneracy of the Wiener index is greater for odd values of *N*, the number of vertices from the molecular graph. The original formula of the Wiener index[25] was extended to afford the computation of the hyper-Wiener index *WW*.[40,41] Because initially *WW* was defined only for acyclic graphs, an extension was proposed for cyclic graphs[42] and a related molecular matrix was defined.[43] The **HyWi** graph operator implements a hyper-Wiener type formula for any molecular matrix;[12,13,23] its weighted graph extension was used to describe the diversity and descriptor clustering for molecules selected from the National Cancer Institute AIDS database.[44,45] Recent developments in the area of distance descriptors include Wiener-related sequences,[46,47] vector−matrix multiplication descriptors,[48] matrix−vector−matrix multiplication descriptors,[49] and novel graph metrics.[50−52] The mean Wiener index for alkanes was computed as an average property of isomeric series;[53,54] this novel concept of mean structural descriptors can be significant in characterizing mixtures of organic compounds. The relatively high degeneracy of *W* due to the global summation of distances can be reduced by using information theory, as demonstrated by the highly discriminating topological indices *U*, *V*, *X*, and *Y* defined on vertex distances.[55−57] Recently, the *U*, *V*, *X*, and *Y* information indices were extended for any symmetric molecular matrix derived from vertex- and edge-weighted molecular graphs,[58,59] giving the graph operators **U**(**M**), **V**(**M**), **X**(**M**), and **Y**(**M**) that were applied with success in QSPR equations[60] and in modeling the retention indices of alkylphenols in gas−liquid chromatography.[61]

In this paper we propose and study a group of novel graph descriptors computed from the graph distances. While in Wiener-like indices all matrix elements are counted together, the main idea is to separate the interatomic distances into two groups, i.e., even and odd graph distances. The even/odd distances are subsequently summed to give two distinct graph invariants that are combined into a series of new graph descriptors that measure the molecular size and shape. These novel descriptors are tested in a large number of QSPR models, and it is demonstrated that such splitting of graph distances into even/odd counts is a fruitful one, offering topological indices with a greater, enhanced correlational power.

EVEN/ODD DISTANCE COUNT STRUCTURAL DESCRIPTORS

Molecular graphs are nondirected chemical graphs that represent organic compounds, using different conventions.[1−15] Usually, only non-hydrogen atoms are taken into account in molecular graphs. In the graph representation of molecules, their geometrical features such as bond lengths or bond angles are not taken into account, and the chemical bonding of atoms is regarded as being their most important characteristic. In molecular graphs vertices correspond to atoms and edges represent covalent bonds between atoms. In this paper we consider only hydrogen-suppressed, simple (nonweighted) molecular graphs, in which vertices correspond to carbon atoms and edges correspond to single carbon−carbon bonds; such molecular graphs are usually used to depict alkanes and cycloalkanes. A graph $G = G(V,E)$ is an ordered pair consisting of two sets, the vertex set $V = V(G)$ and the edge set $E = E(G)$. In a connected graph, the graph distance d_{ij} between a pair of vertices v_i and v_j is equal to the length of the shortest path connecting the two vertices. The graph distance has the following properties: $d_{ii} = 0$ for all $v_i \in V(G)$; $d_{ij} > 0$ for all $v_i \neq v_j$, $v_i, v_j \in V(G)$; $d_{ij} = d_{ji}$ for all $v_i, v_j \in V(G)$; $d_{ik} + d_{kj} \geq d_{ij}$ for all $v_i, v_j, v_k \in V(G)$. For any molecular graph *G*, the element $[D(G)]_{ij}$ of the distance matrix **D** is equal to the topological distance d_{ij} between vertices v_i and v_j.

All elements of the distance matrix **D** can be partitioned into two classes, i.e., even and odd. The sum of even graph distances in the molecular graph *G* is defined with the equation:

$$\mathrm{SumE}(p,G) = \sum_{i<j}^{d_{ij}^{\mathrm{even}}} [D(G)]_{ij}^{p} \qquad (1)$$

where the summation goes over all even elements in the upper triangle of the distance matrix **D** and *p* is a constant that affords an increased flexibility to this graph invariant. When used in QSAR/QSPR models, *p* can be optimized to give better statistical indices. In a similar manner we define the sum of odd graph distances in the molecular graph *G*, by collecting together the remaining graph distances:

$$\mathrm{SumO}(q,G) = \sum_{i<j}^{d_{ij}^{\mathrm{odd}}} [D(G)]_{ij}^{q} \qquad (2)$$

where the summation goes over all odd elements in the upper triangle of the distance matrix **D** and *q* is a constant that weights the odd distances. If $p = q = 1$, the following relationship exists between the Wiener index *W* and the novel indices SumE and SumO:

$$W(G) = \mathrm{SumE}(1,G) + \mathrm{SumO}(1,G) \qquad (3)$$

Both SumE and SumO are graph invariants that can be used as structural descriptors in QSAR/QSPR equations. However, these two indices can be used in the definition of the even−odd sum Wiener index W_{e+o}

$$W_{e+o}(p,q,G) = \mathrm{SumE}(p,G) + \mathrm{SumO}(q,G) \qquad (4)$$

the even−odd ratio Wiener index $W_{e/o}$

$$W_{e/o}(p,q,G) = \frac{\mathrm{SumE}(p,G)}{\mathrm{SumO}(q,G)} \qquad (5)$$

the odd−even ratio Wiener index $W_{o/e}$

$$W_{o/e}(p,q,G) = \frac{\mathrm{SumO}(q,G)}{\mathrm{SumE}(p,G)} \qquad (6)$$

and the even−odd product Wiener index W_{e*o}:

$$W_{e*o}(p,q,G) = \mathrm{SumE}(p,G)\ \mathrm{SumO}(q,G) \qquad (7)$$

Although defined from the graph distances, all structural descriptors proposed here are new. To determine if they represent interesting alternatives to the Wiener-like indices,

in the next section we will investigate the correlational power of the SumE, SumO, W_{e+o}, $W_{e/o}$, $W_{o/e}$, and $W_{e•o}$ indices using QSPR models developed for six alkane properties.

GENERATION OF STRUCTURE−PROPERTY MODELS

Data. The QSPR models were developed for a data set consisting of 134 alkanes between C_6 and C_{10}, for the following six physical properties:[62] t_b, boiling temperature at normal pressure (°C); C_p, molar heat capacity at 300 K (J K^{-1} mol^{-1}); $\Delta_f G°_{300}$(g), standard Gibbs energy of formation in the gas phase at 300 K (kJ mol^{-1}); $\Delta_{vap}H_{300}$, vaporization enthalpy at 300 K (kJ mol^{-1}); $n_D{}^{25}$, refractive index at 25 °C; ρ, density at 25 °C (kg m^{-3}). The value of the refractive index of 2,2,3,3-tetramethylbutane is missing, while the reported density of this compound, 821.70 kg m^{-3}, is seemingly too high when compared with the density of similar alkanes and it was not considered in the computation of the density QSPR models. As is known, there are 142 constitutional isomers for these alkanes, but data for all six properties are missing for the following eight of them: *n*-hexane, *n*-nonane, *n*-decane, 2-methylnonane, 3-methylnonane, 4-methylnonane, 5-methylnonane, and 3-ethyl-2,4-dimethylhexane. This data base of alkane properties was previously used to test a neural network QSPR model, using descriptors derived from the adjacency, distance, and reciprocal distance matrices.[63−66]

Structural Descriptors. The main group of descriptors is represented by the even/odd distance indices SumE(p), SumO(q), $W_{e+o}(p,q)$, $W_{e/o}(p,q)$, $W_{o/e}(p,q)$, and $W_{e•o}(p,q)$. The weighted sum indices SumE(p) and SumO(q) were computed for eight distinct values of the parameters p and q, respectively, i.e. −2, −1.5, −1, −0.5, 0.5, 1, 1.5, and 2. The combined descriptors $W_{e+o}(p,q)$, $W_{e/o}(p,q)$, $W_{o/e}(p,q)$, and $W_{e•o}(p,q)$ were computed for all possible combinations of the parameters p and q.

For comparison purposes, we have also used in the QSPR models several widely employed graph descriptors: the number of carbon atoms N; five Kier and Hall connectivity indices ${}^0\chi$, ${}^1\chi$, ${}^2\chi$, ${}^3\chi_p$, ${}^3\chi_c$;[1,2] four Wiener-like indices computed with the Wiener graph operator **Wi**(**M**), defined via the equation:

$$\mathbf{Wi}(\mathbf{M},G) = \sum_{i=1}^{N}\sum_{j=i}^{N}[\mathbf{M}(G)]_{ij} \qquad (8)$$

where $\mathbf{M} = \mathbf{M}(G)$ is a symmetric $N \times N$ molecular matrix of a molecular graph G with N vertices. The Wiener operator **Wi**(**M**) is an extension of the Wiener index; while W is computed from the distance matrix **D**, the Wiener operator **Wi**(**M**) can be applied to any molecular matrix, derived either from the molecular graph or from the three-dimensional structure of a chemical compound. Four molecular matrices are used in this study for the computation of Wiener-like indices, namely, distance **D**, reciprocal distance **RD**,[28−31] complementary distance **CD**,[35] and reciprocal complementary distance **RCD**[35] matrices.

QSPR Model. Three types of QSAR equations were computed for each alkane property. First, to test the correlational ability of the structural descriptors as shape descriptors, when the molecular size remains constant, we have computed all monoparametric QSPR models for the 18 octane isomers. A second test involved the whole collection of molecules, and its intention was to determine if certain even/odd distance invariants are able to encode in an efficient way both the size and shape (branching) information; in this test only monoparametric correlations were computed. Finally, the third test involved biparametric QSPR models of the entire set of 134 alkanes, in which the size descriptor considered was N and the second descriptor was one of the topological indices investigated in this paper. To make a comparison with the correlational power of well-established topological indices, all QSPR tests will also be performed with connectivity indices and Wiener-like descriptors. For each experiment we will report in the first part of each table the statistical results for the connectivity and Wiener-like indices, with the descriptors in the same order; in the second part of each table we will give the best 15 QSPR equations obtained with the even/odd distance descriptors, ordered according to the decreasing value of F.

Table 1. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with One Independent Variable To Model the Boiling Temperature at Normal Pressure, t_b (°C), of 18 C_8 Alkanes[a]

SD	a_0	a_1	r	s	F
${}^0\chi$	$2.777\,38 \times 10^2$	$-2.488\,25 \times 10$	0.7381	4.27	19.2
${}^1\chi$	2.535 14	$3.049\,36 \times 10$	0.8236	3.59	33.7
${}^2\chi$	$1.440\,98 \times 10^2$	$-9.562\,56$	0.8838	2.96	57.1
${}^3\chi_p$	$1.061\,70 \times 10^2$	4.150 27	0.2925	6.05	1.5
${}^3\chi_c$	$1.205\,09 \times 10^2$	$-7.568\,55$	0.8281	3.55	34.9
Wi(**D**)	$7.805\,82 \times 10$	$5.125\,34 \times 10^{-1}$	0.5407	5.32	6.6
Wi(**RD**)	$2.081\,53 \times 10^2$	$-6.370\,87$	0.5747	5.18	7.9
Wi(**CD**)	$9.700\,11 \times 10$	$1.781\,51 \times 10^{-1}$	0.6236	4.94	10.2
Wi(**RCD**)	$1.297\,82 \times 10^2$	$-1.496\,55$	0.6246	4.94	10.2
$W_{o/e}(-1,-1.5)$	$5.466\,23 \times 10$	$3.637\,56 \times 10$	0.9265	2.38	97.0
$W_{o/e}(-1,-1)$	$5.839\,71 \times 10$	$3.004\,95 \times 10$	0.9240	2.42	93.5
$W_{o/e}(-1.5,-1)$	$6.562\,15 \times 10$	$1.733\,09 \times 10$	0.9202	2.48	88.4
$W_{o/e}(-1,-2)$	$5.378\,84 \times 10$	$3.988\,94 \times 10$	0.9179	2.51	85.6
$W_{e/o}(-1.5,-1)$	$1.579\,40 \times 10^2$	$-1.210\,23 \times 10^2$	0.9163	2.53	83.7
$W_{e/o}(-1,-1.5)$	$1.669\,61 \times 10^2$	$-8.562\,32 \times 10$	0.9153	2.55	82.7
$W_{e/o}(-1,-2)$	$1.695\,27 \times 10^2$	$-8.310\,86 \times 10$	0.9139	2.57	81.1
$W_{o/e}(-1.5,-0.5)$	$7.025\,18 \times 10$	$1.290\,02 \times 10$	0.9131	2.58	80.2
$W_{e/o}(-1.5,-1.5)$	$1.609\,53 \times 10^2$	$-1.141\,71 \times 10^2$	0.9123	2.59	79.4
$W_{o/e}(-1.5,-1.5)$	$6.411\,17 \times 10$	$2.026\,79 \times 10$	0.9101	2.62	77.2
$W_{o/e}(-1,-0.5)$	$6.535\,33 \times 10$	$2.163\,82 \times 10$	0.9064	2.67	73.7
$W_{e/o}(-2,-1)$	$1.541\,25 \times 10^2$	$-1.635\,60 \times 10^2$	0.9059	2.68	73.2
$W_{e/o}(-1,-1)$	$1.613\,85 \times 10^2$	$-8.678\,40 \times 10$	0.9034	2.71	71.0
$W_{o/e}(-2,-0.5)$	$7.442\,28 \times 10$	$7.862\,41$	0.9032	2.72	70.8
$W_{o/e}(-2,-1)$	$7.118\,95 \times 10$	$1.033\,15 \times 10$	0.9028	2.72	70.5

[a] The QSPR models have the general form $t_b = a_0 + a_1$SD.

RESULTS AND DISCUSSION

Normal Boiling Temperature. In Table 1 we present the coefficients and statistical indices for the monoparametric QSPR equations that model the boiling temperature of the 18 octane isomers. The best QSPR model, with $r = 0.9265$, $s = 2.38$, and $F = 97.0$, is obtained with odd/even distance sum index $W_{o/e}(-1,-1.5)$. Moreover, the best 15 even/odd distance descriptors from Table 1 are either $W_{o/e}$ or $W_{e/o}$ indices, suggesting that they encode the molecular shape and branching; these indices are particularly efficient in modeling the octane boiling temperature, since the "traditional" topological indices (connectivity and Wiener-like indices) give inferior QSPR models, with the best results offered by ${}^2\chi$, with $r = 0.8838$, $s = 2.96$, and $F = 57.1$. Another interesting observation regarding the $W_{o/e}$ and $W_{e/o}$ indices

Table 2. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with One Independent Variable To Model the Boiling Temperature at Normal Pressure, t_b (°C), of 134 C_6–C_{10} Alkanes[a]

SD	a_0	a_1	r	s	F
N	$-7.890\,57 \times 10$	$2.385\,93 \times 10$	0.9727	6.19	2314.7
$^0\chi$	$-7.764\,51 \times 10$	$2.896\,89 \times 10$	0.9371	9.30	951.9
$^1\chi$	$-6.604\,31 \times 10$	$4.928\,43 \times 10$	0.9639	7.09	1730.0
$^2\chi$	$6.771\,96 \times 10$	$1.938\,69 \times 10$	0.5336	22.53	52.5
$^3\chi_p$	$6.640\,63 \times 10$	$3.303\,55 \times 10$	0.7329	18.12	153.2
$^3\chi_c$	$1.358\,89 \times 10^2$	3.435 71	0.0860	26.54	1.0
Wi(**D**)	$5.618\,43 \times 10$	$8.047\,04 \times 10^{-1}$	0.9200	10.44	727.2
Wi(**RD**)	4.360 55	7.253 82	0.9522	8.14	1281.9
Wi(**CD**)	$7.809\,71 \times 10$	$4.394\,01 \times 10^{-1}$	0.8053	15.80	243.5
Wi(**RCD**)	$8.710\,01 \times 10$	3.953 90	0.5518	22.22	57.8
Wi(**RW**)	$9.196\,92 \times 10$	$4.667\,84 \times 10^{-1}$	0.7358	18.04	155.8
SumO(−2)	$-3.724\,90 \times 10$	$1.905\,38 \times 10$	0.9804	5.25	3266.3
SumO(−1.5)	$-2.515\,12 \times 10$	$1.620\,11 \times 10$	0.9803	5.26	3253.0
SumO(−1)	−9.090 58	$1.261\,29 \times 10$	0.9786	5.48	2986.0
SumO(−0.5)	9.123 17	8.827 66	0.9743	6.00	2473.1
$W_{e+o}(-2,-0.5)$	8.080 24	7.406 38	0.9679	6.70	1954.9
$W_{e+o}(-1.5,-0.5)$	9.088 93	6.779 59	0.9656	6.93	1819.6
$W_{e+o}(-1,-0.5)$	$1.135\,87 \times 10$	5.927 36	0.9634	7.14	1707.2
$W_{e+o}(-0.5,-0.5)$	$1.572\,11 \times 10$	4.843 67	0.9615	7.32	1614.8
$W_{e+o}(-2,-1)$	−4.262 03	9.742 81	0.9614	7.33	1610.6
$W_{e+o}(-1.5,-1)$	$-7.967\,01 \times 10^{-1}$	8.635 04	0.9563	7.79	1412.8
$W_{e+o}(-0.5,0.5)$	$3.714\,25 \times 10$	2.447 67	0.9560	7.82	1402.0
$W_{e+o}(-2,-1.5)$	$-1.324\,15 \times 10$	$1.162\,61 \times 10$	0.9538	8.00	1331.4
$W_{e+o}(0.5,0.5)$	$4.120\,92 \times 10$	1.622 16	0.9537	8.01	1327.4
$W_{e+o}(-1,-1)$	4.360 48	7.253 82	0.9522	8.14	1281.9
$W_{e+o}(-1,0.5)$	$3.855\,72 \times 10$	2.664 67	0.9506	8.27	1238.8

[a] The QSPR models have the general form $t_b = a_0 + a_1$SD.

from Table 1 is the exclusive presence of negative p and q parameters; therefore, larger graph distances have lower weights and, consequently, a small influence on the value of the graph descriptors. We have to point that the largest contributions to the numerical value of the Wiener index W arises from pairs of distant vertices; on the other hand, in three recently introduced molecular matrices, namely, the reciprocal distance **RD**,[28−31] distance−valency **Dval**,[34] and complementary distance **CD**[35] matrices, the value of the matrix elements corresponding to pairs of vertices decreases when the distance between the vertices increases. Our results from Table 1 obtained with the $W_{o/e}$ and $W_{e/o}$ indices indicate that a good QSPR performance is obtained by structural descriptors that give more weight to shorter graph distances, a property that is consistent with the commonly accepted theory that interactions are inversely proportional to the distance between interacting bodies.

The boiling temperature QSPR models for the entire set of 134 alkanes, obtained with monoparametric equations, are presented in Table 2. In this large set of alkanes, between C_6 and C_{10}, both the size and shape (branching) effects are encountered. The connectivity and Wiener-like indices give worse results than N, because the experimental values of the boiling temperature are clustered according to N, with no overlap between clusters; in this way, a simple size description of the alkane can perform much better than more elaborated structural descriptors. The second part of Table 2 gives the results for the novel even/odd distance descriptors; the weighted sum of odd distances SumO(−2), with $r = 0.9804$, $s = 5.25$, and $F = 3266.3$, is the best one, with much better statistics than N. In fact, the top four positions are occupied by the same index SumO(q) computed with negative values for the parameter q, i.e., $q = -2$, -1.5, -1, and -0.5, while the remaining QSPR equations are obtained with the weighted sum of even and odd distances W_{e+o}. The presence of only negative q parameters in SumO and of almost only negative p and q parameters in W_{e+o} is again an indication that such a distance weighting is more appropriate in good structural descriptors; this can also be noticed by comparing the statistical indices of **Wi**(**D**) and **Wi**(**RD**). However, the separation of even and odd distances in two terms individually weighted gives a higher flexibility and better correlational ability.

The biparametric QSPR equations for the boiling temperature of the entire set of 134 alkanes are presented in Table 3. Since the descriptor N accounts for boiling temperature variations with the molecular size, the second parameter evidently reflects in some way the alkane shape and branching. Basically, we can expect that structural descriptors with good results for the 18 octane set should perform similarly in this instance. Indeed, the best results are obtained by $^2\chi$, with $r = 0.9841$, $s = 4.75$, and $F = 2013.2$; $^2\chi$ represents the weighted contribution of propane-like subgraphs and is a measure of molecular branching. The 15 molecular shape indices $W_{o/e}$ and $W_{e/o}$ offer better QSPR models than the Wiener-like indices, with top results given by $W_{o/e}(-1,-1)$, with $r = 0.9835$, $s = 4.83$, and $F = 1939.3$. Although in this test $^2\chi$ gives slightly better results than $W_{o/e}(-1,-1)$, we have to recall that QSPR equations are statistical models, and a change in the set of molecules can reverse the situation. The important thing is the improvement in QSPR quality when passing from Wiener-like indices to even/odd distance descriptors. A second deduction that can be made regarding the even/odd distance descriptors is their different structural content: while SumE(p), SumO(q), $W_{e+o}(p,q)$, and $W_{e-o}(p,q)$ have a mixed information content regarding both the molecular size and shape, the even−odd ratio indices $W_{e/o}(p,q)$, $W_{o/e}(p,q)$ are mainly shape indices,

Table 3. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with Two Independent Variables To Model the Boiling Temperature at Normal Pressure, t_b (°C), of 134 C_6–C_{10} Alkanes[a]

SD	a_0	a_1	a_2	R	s	F
$^0\chi$	$-7.399\,40 \times 10$	$3.407\,21 \times 10$	$-1.312\,69 \times 10$	0.9762	5.80	1329.4
$^1\chi$	$-7.851\,66 \times 10$	$1.448\,77 \times 10$	$2.047\,59 \times 10$	0.9800	5.32	1591.4
$^2\chi$	$-8.179\,87 \times 10$	$2.712\,05 \times 10$	$-7.27\,719$	0.9841	4.75	2013.2
$^3\chi_p$	$-7.073\,22 \times 10$	$2.097\,21 \times 10$	$8.246\,95$	0.9827	4.95	1842.7
$^3\chi_c$	$-7.980\,26 \times 10$	$2.458\,52 \times 10$	$-5.369\,99$	0.9815	5.13	1717.3
Wi(**D**)	$-8.947\,48 \times 10$	$2.585\,99 \times 10$	$-7.479\,41 \times 10^{-2}$	0.9730	6.17	1163.6
Wi(**RD**)	$-8.804\,19 \times 10$	$2.665\,52 \times 10$	$-8.833\,26e \times 10^{-1}$	0.9729	6.19	1158.9
Wi(**CD**)	$-7.470\,83 \times 10$	$2.307\,26 \times 10$	$2.149\,07 \times 10^{-2}$	0.9729	6.18	1160.5
Wi(**RCD**)	$-8.147\,36 \times 10$	$2.478\,44 \times 10$	$-4.448\,11 \times 10$	0.9739	6.07	1205.9
Wi(**RW**)	$-7.524\,88 \times 10$	$2.320\,53 \times 10$	$2.286\,50 \times 10^{-2}$	0.9730	6.18	1162.0
$W_{o/e}(-1,-1)$	$-1.385\,77 \times 10^2$	$2.578\,69 \times 10$	$2.402\,07 \times 10$	0.9835	4.83	1939.3
$W_{e/o}(-1,-1)$	$-5.548\,06 \times 10$	$2.538\,27 \times 10$	$-6.464\,49 \times 10$	0.9831	4.90	1886.3
$W_{e/o}(-0.5,-1.5)$	$-6.513\,70 \times 10$	$2.728\,00 \times 10$	$-4.297\,41 \times 10$	0.9831	4.90	1883.6
$W_{o/e}(-1,-1.5)$	$-1.489\,06 \times 10^2$	$2.672\,97 \times 10$	$2.885\,40 \times 10$	0.9829	4.92	1871.6
$W_{o/e}(-1.5,-1)$	$-1.260\,00 \times 10^2$	$2.496\,56 \times 10$	$1.380\,43 \times 10$	0.9829	4.92	1867.1
$W_{o/e}(-1,-0.5)$	$-1.211\,34 \times 10^2$	$2.450\,15 \times 10$	$1.666\,14 \times 10$	0.9829	4.92	1866.2
$W_{e/o}(-1,-1.5)$	$-5.953\,15 \times 10$	$2.625\,59 \times 10$	$-6.185\,03 \times 10$	0.9829	4.93	1864.8
$W_{o/e}(-0.5,-1)$	$-1.497\,00 \times 10^2$	$2.680\,80 \times 10$	$3.925\,56 \times 10$	0.9828	4.93	1859.3
$W_{e/o}(-0.5,-1)$	$-6.106\,09 \times 10$	$2.615\,97 \times 10$	$-4.286\,16 \times 10$	0.9828	4.94	1855.7
$W_{e/o}(-0.5,-2)$	$-6.870\,07 \times 10$	$2.800\,00 \times 10$	$-4.191\,65 \times 10$	0.9826	4.96	1836.3
$W_{e/o}(-1.5,-1)$	$-5.318\,48 \times 10$	$2.474\,20 \times 10$	$-8.945\,06 \times 10$	0.9826	4.97	1830.5
$W_{o/e}(-1.5,-0.5)$	$-1.123\,65 \times 10^2$	$2.393\,62 \times 10$	$9.804\,06$	0.9825	4.99	1818.2
$W_{o/e}(-0.5,-1.5)$	$-1.631\,89 \times 10^2$	$2.795\,86 \times 10$	$4.836\,26 \times 10$	0.9824	5.00	1808.7
$W_{o/e}(-0.5,-0.5)$	$-1.297\,50 \times 10^2$	$2.530\,09 \times 10$	$2.707\,67 \times 10$	0.9823	5.00	1805.1
$W_{e/o}(-1,-0.5)$	$-5.264\,96 \times 10$	$2.429\,82 \times 10$	$-6.523\,02 \times 10$	0.9822	5.02	1793.4

[a] The QSPR models have the general form $t_b = a_0 + a_1N + a_2$SD, where N is the number of carbon atoms.

as demonstrated by their good results both for octanes and, in combination with N, for the entire set of alkanes. A certain preference for the sum of odd distances SumO(q) was noticed, but it remains to be demonstrated if this has a larger significance or is limited only to boiling temperature.

Molar Heat Capacity. As one can see from the results reported in Table 4, no single index is able to model well the alkane molar heat capacity of the 18 octane isomers. We do not claim that such a descriptor does not exist, but it is not found in the set of topological indices tested in this paper. The results presented in Table 5 show that for the entire set of 134 alkanes the number of carbon atoms N is the best descriptor (with $r = 0.9870$, $s = 4.10$, and $F = 4977.7$) followed by the sum of odd distances SumO(-2) (with $r = 0.9797$, $s = 5.10$, and $F = 3160.6$). Overall, the novel even/odd distance descriptors give better results than the connectivity and Wiener-like indices. We have to point out here the identity of two descriptors that appear in Table 5, namely, **Wi**(**RD**) and $W_{e+o}(-1,-1)$: both are the sum of the reciprocal values of all distances in the molecular graph. It is worth pointing out that only size and shape indices SumO(q) and $W_{e+o}(p,q)$ are present in Table 5, generally with negative values for the parameters p and q. The results from Table 6, representing biparametric QSPR models for the 134 alkane molar heat capacity, show that the first places are occupied by $W_{e+o}(-2,0.5)$, with $r = 0.9874$, $s = 4.05$, and $F = 2545.2$, and $^1\chi$, with $r = 0.9873$, $s = 4.06$, and $F = 2539.8$. All these biparametric equations that contain N and a graph descriptor offer only a marginal improvement over the monoparametric QSPR model with N, presented in Table 5. Although the alkane molar heat capacity cannot be adequately modeled only with the investigated descriptors and with such simple models, the even/odd distance descriptors are comparable to the other conventional descriptors considered.

Table 4. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with One Independent Variable To Model the Molar Heat Capacity at 300 K, C_p (J K^{-1} mol^{-1}), of 18 C_8 Alkanes[a]

SD	a_0	a_1	r	s	F
$^0\chi$	$1.832\,99 \times 10^2$	$8.389\,27 \times 10^{-1}$	0.0546	2.88	<0.1
$^1\chi$	$1.9134\,8 \times 10^2$	$-6.909\,35 \times 10^{-1}$	0.0409	2.88	<0.1
$^2\chi$	$1.881\,00 \times 10^2$	$2.296\,04 \times 10^{-1}$	0.0466	2.88	<0.1
$^3\chi_p$	$1.899\,30 \times 10^2$	$-6.059\,70 \times 10^{-1}$	0.0937	2.87	0.1
$^3\chi_c$	$1.886\,41 \times 10^2$	$2.094\,68 \times 10^{-1}$	0.0503	2.88	<0.1
Wi(**D**)	$1.918\,96 \times 10^2$	$-4.409\,39 \times 10^{-2}$	0.1021	2.87	0.2
Wi(**RD**)	$1.831\,16 \times 10^2$	$3.854\,14 \times 10^{-1}$	0.0763	2.87	0.1
Wi(**CD**)	$1.914\,27 \times 10^2$	$-2.770\,23 \times 10^{-2}$	0.2128	2.82	0.8
Wi(**RCD**)	$1.862\,72 \times 10^2$	$2.381\,06 \times 10^{-1}$	0.2180	2.81	0.8
$W_{o/e}(0.5,1)$	$1.953\,12 \times 10^2$	$-3.743\,61$	0.4100	2.63	3.2
$W_{o/e}(1,1.5)$	$1.939\,87 \times 10^2$	$-2.925\,02$	0.4042	2.64	3.1
$W_{o/e}(0.5,0.5)$	$1.959\,43 \times 10^2$	$-6.490\,41$	0.3889	2.66	2.9
$W_{o/e}(0.5,1.5)$	$1.938\,17 \times 10^2$	$-1.696\,05$	0.3930	2.65	2.9
$W_{o/e}(1,2)$	$1.929\,08 \times 10^2$	$-1.292\,91$	0.3869	2.66	2.8
$W_{o/e}(1.5,2)$	$1.927\,90 \times 10^2$	$-2.156\,56$	0.3843	2.66	2.8
$W_{o/e}(1,1)$	$1.942\,79 \times 10^2$	$-5.232\,26$	0.3819	2.66	2.7
$W_{e+o}(-2,0.5)$	$2.022\,02 \times 10^2$	$-5.441\,31 \times 10^{-1}$	0.3650	2.68	2.5
$W_{e+o}(-1.5,0.5)$	$2.035\,54 \times 10^2$	$-5.727\,86 \times 10^{-1}$	0.3676	2.68	2.5
$W_{e+o}(-1,0.5)$	$2.058\,63 \times 10^2$	$-6.202\,57 \times 10^{-1}$	0.3696	2.68	2.5
$W_{e+o}(-0.5,0.5)$	$2.102\,40 \times 10^2$	$-7.074\,50 \times 10^{-1}$	0.3689	2.68	2.5
$W_{o/e}(1.5,1.5)$	$1.928\,92 \times 10^2$	$-3.940\,61$	0.3628	2.69	2.4
SumO(0.5)	$1.994\,64 \times 10^2$	$-4.787\,55 \times 10^{-1}$	0.3514	2.70	2.3
$W_{o/e}(-0.5,0.5)$	$1.952\,27 \times 10^2$	$-2.291\,97$	0.3538	2.70	2.3
$W_{o/e}(0.5,2)$	$1.923\,46 \times 10^2$	$-6.661\,27 \times 10^{-1}$	0.3564	2.69	2.3

[a] The QSPR models have the general form $C_p = a_0 + a_1$SD.

Standard Gibbs Energy of Formation. The alkane standard Gibbs energy of formation is also a somewhat difficult property to model only with the descriptors involved in this study, as can be seen from the results from Table 7 obtained for the 18 octane isomers. The top results are obtained with $^3\chi_p$ ($r = 0.7951$, $s = 2.39$, and $F = 27.5$) and SumO(-2) ($r = 0.7855$, $s = 2.44$, and $F = 25.8$). A total of three SumO descriptors are present in Table 7, all three with

Table 5. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with One Independent Variable To Model the Molar Heat Capacity at 300 K, C_p (J K^{-1} mol^{-1}), of 134 C_6–C_{10} Alkanes[a]

SD	a_0	a_1	r	s	F
N	3.689 19	2.316 10 × 10	0.9870	4.10	4977.7
$^0\chi$	2.212 96	2.848 11 × 10	0.9631	6.86	1691.9
$^1\chi$	2.202 03 × 10	4.644 08 × 10	0.9495	8.00	1208.2
$^2\chi$	1.337 92 × 10^2	2.211 96 × 10	0.6364	19.66	89.9
$^3\chi_p$	1.558 40 × 10^2	2.706 00 × 10	0.6276	19.84	85.8
$^3\chi_c$	2.078 49e × 10^2	7.396 00	0.1936	25.00	5.1
Wi(**D**)	1.341 37 × 10^2	7.877 90 × 10^{-1}	0.9415	8.59	1030.1
Wi(**RD**)	8.431 97 × 10	7.052 16	0.9677	6.43	1943.9
Wi(**CD**)	1.567 88 × 10^2	4.215 99 × 10^{-1}	0.8077	15.03	247.7
Wi(**RCD**)	1.628 21 × 10^2	3.990 02	0.5820	20.72	67.6
Wi(**RW**)	1.702 91 × 10^2	4.459 82 × 10^{-1}	0.7349	17.28	155.0
SumO(−2)	4.673 15 × 10	1.821 54 × 10	0.9797	5.10	3160.6
$W_{e+o}(-0.5,-0.5)$	9.528 67 × 10	4.712 06	0.9778	5.34	2869.6
SumO(−1.5)	5.921 88 × 10	1.539 75 × 10	0.9739	5.78	2433.7
$W_{e+o}(0.5,0.5)$	1.197 16 × 10^2	1.584 12	0.9736	5.82	2399.5
$W_{e+o}(-0.5,-1)$	9.049 72 × 10	5.548 33	0.9726	5.93	2307.8
$W_{e+o}(-1,-0.5)$	9.200 72 × 10	5.721 71	0.9722	5.97	2275.2
$W_{e+o}(0.5,-0.5)$	1.132 90 × 10^2	2.310 28	0.9708	6.11	2165.5
$W_{e+o}(-0.5,-1.5)$	8.787 12 × 10	6.102 20	0.9683	6.37	1981.1
$W_{e+o}(-1.5,-0.5)$	9.062 72 × 10	6.502 24	0.9681	6.39	1969.4
$W_{e+o}(-1,-1)$	8.431 97 × 10	7.052 16	0.9677	6.43	1943.9
SumO(−1)	7.520 95 × 10	1.192 57 × 10	0.9672	6.47	1916.5
$W_{e+o}(-2,-0.5)$	9.027 57 × 10	7.068 69	0.9656	6.63	1821.1
$W_{e+o}(-0.5,-2)$	8.647 15 × 10	6.441 70	0.9656	6.63	1818.4
$W_{e+o}(-1.5,-1)$	8.026 45 × 10	8.336 01	0.9651	6.68	1791.0
$W_{e+o}(-2,-1)$	7.771 22 × 10	9.351 70	0.9646	6.72	1767.8

[a] The QSPR models have the general form $C_p = a_0 + a_1$SD.

Table 6. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with Two Independent Variables To Model the Molar Heat Capacity at 300 K, C_p (J K^{-1} mol^{-1}), of 134 C_6–C_{10} Alkanes[a]

SD	a_0	a_1	a_2	r	s	F
$^0\chi$	4.983 14	2.585 14 × 10	−3.458 17	0.9873	4.07	2523.1
$^1\chi$	3.770 76	2.119 65 × 10	4.292 18	0.9873	4.06	2539.8
$^2\chi$	3.226 20	2.368 29 × 10	−1.164 66	0.9873	4.06	2533.2
$^3\chi_p$	3.155 38	2.334 95 × 10	−5.386 10 × 10^{-1}	0.9870	4.10	2479.0
$^3\chi_c$	3.531 30	2.328 88 × 10	−9.453 58 × 10^{-1}	0.9873	4.07	2528.5
Wi(**D**)	3.821 98	2.313 58 × 10	9.396 54 × 10^{-4}	0.9870	4.11	2470.0
Wi(**RD**)	−1.915 31	2.487 60 × 10	−5.418 64 × 10^{-1}	0.9871	4.10	2488.4
Wi(**CD**)	4.899 45	2.293 41 × 10	6.196 48 × 10^{-3}	0.9870	4.11	2474.6
Wi(**RCD**)	2.585 95	2.355 84 × 10	−1.911 07 × 10^{-1}	0.9872	4.07	2519.0
Wi(**RW**)	4.717 55	2.297 71 × 10	6.42994 × 10^{-3}	0.9870	4.11	2475.0
$W_{e\cdot o}(-2,0.5)$	−9.624 01	2.529 98 × 10	−6.525 45 × 10^{-2}	0.9874	4.05	2545.2
$W_{e\cdot o}(-1.5,0.5)$	−9.861 83	2.532 21 × 10	−4.312 74 × 10^{-2}	0.9873	4.06	2533.7
$W_{e\cdot o}(-2,1)$	−7.624 33	2.493 22 × 10	−3.058 87 × 10^{-2}	0.9873	4.06	2530.6
$W_{e\cdot o}(-2,-0.5)$	−5.176 04	2.467 80 × 10	−1.104 60 × 10^{-1}	0.9873	4.07	2525.5
$W_{e\cdot o}(-2,-1)$	−3.804 35	2.448 26 × 10	−1.273 72 × 10^{-1}	0.9872	4.07	2518.4
$W_{e\cdot o}(-1.5,-0.5)$	−5.711 69	2.475 17 × 10	−7.550 09 × 10^{-2}	0.9872	4.07	2518.2
$W_{e\cdot o}(-1,0.5)$	−9.470 48	2.524 06 × 10	−2.644 50 × 10^{-2}	0.9872	4.07	2518.0
$W_{e\cdot o}(-1.5,1)$	−6.797 66	2.479 31 × 10	−1.846 05 × 10^{-2}	0.9872	4.07	2517.1
$W_{e\cdot o}(-2,-1.5)$	−3.147 59	2.439 61 × 10	−1.436 65 × 10^{-1}	0.9872	4.08	2514.8
$W_{e\cdot o}(-2,-2)$	−2.858 17	2.436 37 × 10	−1.574 19 × 10^{-1}	0.9872	4.08	2513.0
$W_{e\cdot o}(-1.5,-1)$	−4.172 46	2.452 93 × 10	−8.580 59 × 10^{-2}	0.9872	4.08	2511.1
$W_{e\cdot o}(-1,-0.5)$	−6.367 29	2.483 95 × 10	−5.055 14 × 10^{-2}	0.9872	4.08	2508.9
$W_{e\cdot o}(-2,1.5)$	−3.510 74	2.426 48 × 10	−1.012 23 × 10^{-2}	0.9872	4.08	2507.6
$W_{e\cdot o}(-1.5,-1.5)$	−3.412 55	2.442 48 × 10	−9.552 46 × 10^{-2}	0.9872	4.08	2507.2
$W_{e\cdot o}(-1.5,-2)$	−3.055 16	2.437 98 × 10	−1.035 64 × 10^{-1}	0.9872	4.08	2505.0

[a] The QSPR models have the general form $C_p = a_0 + a_1N + a_2$SD, where N is the number of carbon atoms.

negative values for the parameter q; similarly to the results obtained for the boiling temperature (Table 2) and molar heat capacity (Table 5), it seems that the sum of odd distances has a greater structural relevance than the sum of even distances. Another group of even/odd distance descriptors relevant to the modeling of octane $\Delta_f G°_{300}$ is represented by several $W_{e+o}(p,q)$, mainly with negative p and q parameters.

The standard Gibbs energy of formation QSPR models for the entire set of 134 alkanes, obtained with monoparametric equations, are presented in Table 8. Although the size parameter N ($r = 0.8008$, $s = 8.85$, and $F = 236.0$) has a dominant role in this data set, the best results are obtained with an even/odd index that incorporates both size and shape information, namely, $W_{e\cdot o}(-2,-1)$, with $r = 0.8889$, $s = 6.77$,

Table 7. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with One Independent Variable To Model the Standard Gibbs Energy of Formation in the Gas Phase at 300 K, $\Delta_f G°_{300}$(g) (kJ mol^{-1}), of 18 C_8 Alkanes[a]

SD	a_0	a_1	r	s	F
$^0\chi$	$-4.112\,90 \times 10$	8.878 27	0.4232	3.57	3.5
$^1\chi$	$4.039\,45 \times 10$	$-6.307\,64$	0.2738	3.79	1.3
$^2\chi$	$1.497\,79 \times 10$	$7.616\,09 \times 10^{-1}$	0.1131	3.91	0.2
$^3\chi_p$	4.648 79	7.019 66	0.7951	2.39	27.5
$^3\chi_c$	$1.621\,67 \times 10$	1.314 93	0.2312	3.83	0.9
Wi(**D**)	$4.253\,63 \times 10$	$-3.614\,08 \times 10^{-1}$	0.6128	3.11	9.6
Wi(**RD**)	$-4.432\,24 \times 10$	4.163 40	0.6036	3.14	9.2
Wi(**CD**)	$2.669\,85 \times 10$	$-9.917\,20 \times 10^{-2}$	0.5579	3.27	7.2
Wi(**RCD**)	8.424 33	$8.355\,11 \times 10^{-1}$	0.5604	3.26	7.3
SumO(−2)	$-1.666\,47 \times 10^2$	$2.354\,08 \times 10$	0.7855	2.44	25.8
SumO(−1.5)	$-9.931\,06 \times 10$	$1.381\,62 \times 10$	0.7409	2.64	19.5
$W_{e+o}(-2,-1)$	$-5.236\,30 \times 10$	5.843 62	0.7067	2.78	16.0
$W_{e+o}(-1.5,-1)$	$-4.817\,05 \times 10$	5.017 15	0.6712	2.92	13.1
$W_{e+o}(-1,-0.5)$	$-5.796\,48 \times 10$	4.469 35	0.6697	2.92	13.0
$W_{e+o}(-1.5,-0.5)$	$-4.833\,29 \times 10$	4.351 18	0.6682	2.93	12.9
$W_{e+o}(-2,-1.5)$	$-5.008\,63 \times 10$	6.242 39	0.6565	2.97	12.1
SumO(−1)	$-5.581\,82 \times 10$	7.646 95	0.6554	2.97	12.0
$W_{e+o}(-2,-0.5)$	$-4.282\,34 \times 10$	4.309 06	0.6509	2.99	11.8
$W_{e+o}(0.5,0.5)$	$7.668\,56 \times 10$	$-1.386\,87$	0.6165	3.10	9.8
$W_{e+o}(-0.5,-0.5)$	$-7.509\,57 \times 10$	4.703 76	0.6114	3.11	9.6
$W_{e+o}(1,1)$	$4.253\,63 \times 10$	$-3.614\,08 \times 10^{-1}$	0.6128	3.11	9.6
$W_{e+o}(-1,-1)$	$-4.432\,24 \times 10$	4.163 40	0.6036	3.14	9.2
$W_{e+o}(1.5,1.5)$	$3.200\,71 \times 10$	$-1.221\,67 \times 10^{-1}$	0.6047	3.13	9.2
$W_{o/e}(1.5,-1)$	8.557 21	$5.268\,41 \times 10$	0.6002	3.15	9.0

[a] The QSPR models have the general form $\Delta_f G°_{300} = a_0 + a_1$SD.

Table 8. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with One Independent Variable To Model the Standard Gibbs Energy of Formation in the Gas Phase at 300 K, $\Delta_f G°_{300}$(g) (kJ mol^{-1}), of 134 C_6–C_{10} Alkanes[a]

SD	a_0	a_1	r	s	F
N	$-6.989\,57 \times 10$	$1.089\,60 \times 10$	0.8008	8.85	236.0
$^0\chi$	$-7.864\,97 \times 10$	$1.447\,37 \times 10$	0.8441	7.92	327.2
$^1\chi$	$-5.397\,07 \times 10$	$2.009\,79 \times 10$	0.7087	10.43	133.2
$^2\chi$	$-1.410\,51 \times 10$	$1.186\,76 \times 10$	0.5889	11.94	70.1
$^3\chi_p$	$-1.546\,62 \times 10$	$2.047\,42 \times 10$	0.8189	8.48	268.8
$^3\chi_c$	$2.258\,19 \times 10$	6.812 51	0.3076	14.06	13.8
Wi(**D**)	$-1.809\,35$	$3.057\,88 \times 10^{-1}$	0.6303	11.47	87.0
Wi(**RD**)	$-3.863\,65 \times 10$	3.675 69	0.8699	7.29	410.5
Wi(**CD**)	$1.274\,93 \times 10$	$1.224\,27 \times 10^{-1}$	0.4045	13.51	25.8
Wi(**RCD**)	$-1.227\,61 \times 10$	3.176 57	0.7992	8.88	233.3
Wi(**RW**)	$1.896\,08 \times 10$	$1.070\,45 \times 10^{-1}$	0.3042	14.08	13.5
$W_{e\cdot o}(-2,-1)$	$-9.405\,48$	1.085 67	0.8889	6.77	497.2
$W_{e\cdot o}(-2,-1.5)$	$-1.074\,61 \times 10$	1.304 64	0.8887	6.78	495.7
$W_{e\cdot o}(-1.5,-1)$	$-8.982\,79$	$7.143\,82 \times 10^{-1}$	0.8865	6.84	484.7
$W_{e\cdot o}(-1.5,-1.5)$	$-1.027\,86 \times 10$	$8.578\,98 \times 10^{-1}$	0.8863	6.84	483.4
$W_{e\cdot o}(-2,-2)$	$-1.151\,27 \times 10$	1.458 88	0.8839	6.91	471.3
$W_{e\cdot o}(-1.5,-2)$	$-1.099\,25 \times 10$	$9.583\,28 \times 10^{-1}$	0.8813	6.98	459.1
$W_{e\cdot o}(-1,-1)$	$-8.148\,06$	$4.550\,97 \times 10^{-1}$	0.8788	7.05	447.7
$W_{e\cdot o}(-2,-0.5)$	$-7.332\,88$	$8.178\,69 \times 10^{-1}$	0.8785	7.06	446.3
$W_{e\cdot o}(-1,-1.5)$	−9.360pb05	$5.458\,08 \times 10^{-1}$	0.8784	7.06	445.7
$W_{e+o}(-1.5,-1.5)$	$-4.550\,32 \times 10$	5.150 22	0.8757	7.14	434.1
$W_{e\cdot o}(-1.5,-0.5)$	$-6.926\,15$	$5.379\,71 \times 10^{-1}$	0.8756	7.14	433.8
$W_{e+o}(-2,-1.5)$	$-4.786\,58 \times 10$	5.914 81	0.8749	7.16	430.6
$W_{e\cdot o}(-1,-2)$	$-9.986\,60$	$6.086\,42 \times 10^{-1}$	0.8730	7.21	422.7
$W_{e+o}(-1.5,-1)$	$-4.109\,05 \times 10$	4.365 80	0.8717	7.24	417.7
$W_{e+o}(-1.5,-2)$	$-4.779\,75 \times 10$	5.649 46	0.8716	7.24	417.4

[a] The QSPR models have the general form $\Delta_f G°_{300} = a_0 + a_1$SD.

and $F = 497.2$. In the group of the 15 best even/odd descriptors there are 11 $W_{e\cdot o}(p,q)$ indices and 4 $W_{e+o}(p,q)$ indices, all computed with negative p and q parameters; all 15 even/odd descriptors give modestly better results than the connectivity and Wiener-like indices. When used together with N, the distance sum indices $W_{e+o}(p,q)$ with positive p and q parameters give the best QSPR models, as one can see from Table 9; the top index is $W_{e+o}(1.5,2)$, with $r = 0.9274$, $s = 5.55$, and $F = 402.6$. A comparison with the first part of Table 9, containing QSPR equations obtained with the reference indices, shows again a superiority for the even/odd distance descriptors.

Vaporization Enthalpy. The size-independent QSPR models for the vaporization enthalpy of the 18 octane isomers are presented in Table 10. From the best 15 even/odd distance descriptors, the first 11 are distance product indices $W_{e\cdot o}$-

Table 9. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with Two Independent Variables To Model the Standard Gibbs Energy of Formation in the Gas Phase at 300 K, $\Delta_f G°_{300}$(g) (kJ mol^{-1}), of 134 C_6–C_{10} Alkanes[a]

SD	a_0	a_1	a_2	r	s	F
$^0\chi$	$-7.965\,70 \times 10$	$-9.400\,44$	$2.608\,79 \times 10$	0.8550	7.69	178.1
$^1\chi$	$-7.022\,72 \times 10$	$1.888\,17 \times 10$	$-1.744\,78 \times 10$	0.8218	8.45	136.2
$^2\chi$	$-6.907\,49 \times 10$	$9.970\,75$	$2.064\,69$	0.8045	8.81	120.1
$^3\chi_p$	$-5.705\,42 \times 10$	$6.359\,92$	$1.295\,69 \times 10$	0.8937	6.65	260.0
$^3\chi_c$	$-6.938\,49 \times 10$	$1.048\,27 \times 10$	$3.057\,91$	0.8121	8.66	126.8
Wi(**D**)	$-1.713\,03 \times 10^2$	$3.009\,14 \times 10$	$-7.176\,24 \times 10^{-1}$	0.9159	5.96	340.8
Wi(**RD**)	$3.715\,33 \times 10$	$-2.186\,29 \times 10$	$1.034\,99 \times 10$	0.9186	5.86	353.9
Wi(**CD**)	$-1.133\,33 \times 10^2$	$1.903\,76 \times 10$	$-2.223\,98 \times 10^{-1}$	0.9073	6.24	305.0
Wi(**RCD**)	$-5.852\,42 \times 10$	$6.799\,58$	$1.969\,79$	0.8923	6.70	255.9
Wi(**RW**)	$-1.057\,07 \times 10^2$	$1.730\,05 \times 10$	$-2.239\,14 \times 10^{-1}$	0.9081	6.21	308.0
$W_{e+o}(1.5,2)$	$-1.287\,62 \times 10^2$	$2.108\,71 \times 10$	$-1.276\,21 \times 10^{-1}$	0.9274	5.55	402.6
$W_{e+o}(1,1.5)$	$-1.458\,47 \times 10^2$	$2.468\,88 \times 10$	$-3.482\,74 \times 10^{-1}$	0.9250	5.64	388.0
$W_{e+o}(2,2)$	$-1.269\,62 \times 10^2$	$2.066\,37 \times 10$	$-9.127\,61 \times 10^{-2}$	0.9235	5.69	379.5
$W_{e+o}(1,2)$	$-1.241\,20 \times 10^2$	$2.030\,96 \times 10$	$-1.407\,45 \times 10^{-1}$	0.9223	5.73	373.2
$W_{e+o}(1.5,1.5)$	$-1.429\,40 \times 10^2$	$2.395\,44 \times 10$	$-2.483\,84 \times 10^{-1}$	0.9221	5.74	372.2
$W_{e+o}(-2,-1.5)$	$4.743\,68$	$-1.907\,30 \times 10$	$1.519\,97 \times 10$	0.9189	5.85	355.2
$W_{e+o}(-1,-1)$	$3.715\,39 \times 10$	$-2.186\,31 \times 10$	1.03499×10	0.9186	5.86	353.9
$W_{e+o}(0.5,2)$	$-1.198\,60 \times 10^2$	$1.955\,19 \times 10$	$-1.429\,82 \times 10^{-1}$	0.9179	5.89	350.4
$W_{e+o}(0.5,1.5)$	$-1.374\,37 \times 10^2$	$2.322\,05 \times 10$	$-3.705\,78 \times 10^{-1}$	0.9162	5.94	342.5
$W_{e+o}(-1.5,-1.5)$	$6.734\,34$	$-1.759\,90 \times 10$	$1.259\,15 \times 10$	0.9160	5.95	341.3
$W_{e+o}(1,1)$	$-1.713\,03 \times 10^2$	$3.009\,14 \times 10$	$-7.176\,24 \times 10^{-1}$	0.9159	5.96	340.8
$W_{e+o}(-1.5,-1)$	$2.287\,95 \times 10$	$-1.945\,69 \times 10$	$1.139\,07 \times 10$	0.9151	5.98	337.2
$W_{e+o}(-0.5,2)$	$-1.158\,54e \times 10^2$	$1.879\,98e \times 10$	$-1.419\,35e \times 10^{-1}$	0.9147	6.00	335.4
$W_{e+o}(-1,2)$	$-1.150\,66 \times 10^2$	$1.864\,12 \times 10$	$-1.413\,56 \times 10^{-1}$	0.9143	6.01	333.7
$W_{e+o}(-1.5,2)$	$-1.146\,22 \times 10^2$	$1.854\,75 \times 10$	$-1.409\,34 \times 10^{-1}$	0.9141	6.01	333.1

[a] The QSPR models have the general form $\Delta_f G°_{300} = a_0 + a_1 N + a_2$SD, where N is the number of carbon atoms.

Table 10. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with One Independent Variable To Model the Vaporization Enthalpy at 300 K, $\Delta_{vap}H_{300}$ (kJ mol^{-1}), of 18 C_8 Alkanes[a]

SD	a_0	a_1	r	s	F
$^0\chi$	$8.819\,61 \times 10$	$-8.242\,14$	0.8977	0.76	66.4
$^1\chi$	$3.623\,46$	$8.294\,21$	0.8225	0.98	33.5
$^2\chi$	$4.056\,21 \times 10$	$-2.108\,22$	0.7154	1.20	16.8
$^3\chi_p$	$3.700\,68 \times 10$	$-1.731\,35$	0.4480	1.54	4.0
$^3\chi_c$	$3.545\,67 \times 10$	$-1.774\,36$	0.7128	1.21	16.5
Wi(**D**)	$1.796\,93 \times 10$	$2.284\,92 \times 10^{-1}$	0.8851	0.80	57.9
Wi(**RD**)	$7.303\,18 \times 10$	$-2.642\,20$	0.8751	0.83	52.3
Wi(**CD**)	$2.798\,58 \times 10$	$6.266\,38 \times 10^{-2}$	0.8054	1.02	29.5
Wi(**RCD**)	$3.857\,19 \times 10$	$-4.384\,90 \times 10^{-1}$	0.6719	1.28	13.2
$W_{e•o}(2,1)$	$2.945\,00 \times 10$	$1.156\,78 \times 10^{-3}$	0.9087	0.72	75.8
$W_{e•o}(1.5,1)$	$2.813\,49 \times 10$	$2.719\,73 \times 10^{-3}$	0.9086	0.72	75.7
$W_{e•o}(2,1.5)$	$3.018\,13 \times 10$	$5.618\,31 \times 10^{-4}$	0.9084	0.72	75.6
$W_{e•o}(1.5,1.5)$	$2.934\,03 \times 10$	$1.254\,63 \times 10$	0.9023	0.74	70.1
$W_{e•o}(2,2)$	$3.081\,82 \times 10$	$2.550\,95 \times 10^{-4}$	0.9017	0.74	69.6
$W_{e•o}(1,0.5)$	$2.347\,06 \times 10$	$1.364\,48 \times 10^{-2}$	0.8997	0.75	68.0
$W_{e•o}(1,1)$	$2.618\,90 \times 10$	$6.360\,17 \times 10^{-3}$	0.8984	0.76	67.0
$W_{e•o}(1.5,0.5)$	$2.690\,04 \times 10$	$5.250\,05 \times 10^{-3}$	0.8980	0.76	66.6
$W_{e•o}(2,0.5)$	$2.878\,02 \times 10$	$2.121\,78 \times 10^{-3}$	0.8954	0.77	64.7
$W_{e•o}(1.5,2)$	$3.027\,89 \times 10$	$5.481\,90 \times 10^{-4}$	0.8916	0.78	62.0
$W_{e•o}(0.5,0.5)$	$1.626\,04 \times 10$	$3.880\,20 \times 10^{-2}$	0.8891	0.79	60.4
$W_{e+o}(2,2)$	$2.747\,20 \times 10$	$2.967\,59 \times 10^{-2}$	0.8881	0.79	59.8
$W_{e+o}(1.5,1.5)$	$2.448\,42 \times 10$	$7.842\,48 \times 10^{-2}$	0.8869	0.80	58.9
$W_{e+o}(1,1)$	$1.796\,93 \times 10$	$2.284\,92 \times 10^{-1}$	0.8851	0.80	57.9
$W_{e+o}(0.5,0.5)$	$-3.306\,86$	$8.694\,71 \times 10^{-1}$	0.8830	0.81	56.6

[a] The QSPR models have the general form $\Delta_{vap}H_{300} = a_0 + a_1$SD.

Table 11. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with One Independent Variable To Model the Vaporization Enthalpy at 300 K, $\Delta_{vap}H_{300}$ (kJ mol^{-1}), of 134 C_6–C_{10} Alkanes[a]

SD	a_0	a_1	r	s	F
N	$4.194\,65$	$3.700\,44$	0.9303	1.58	849.5
$^0\chi$	$6.229\,51$	$4.247\,59$	0.8474	2.29	336.3
$^1\chi$	$4.234\,69$	$8.112\,28$	0.9785	0.89	2968.0
$^2\chi$	$2.885\,48 \times 10$	$2.488\,87$	0.4225	3.92	28.7
$^3\chi_p$	$2.999\,32 \times 10$	$3.650\,88$	0.4995	3.74	43.9
$^3\chi_c$	$3.839\,53 \times 10$	$-2.959\,12 \times 10^{-1}$	0.0457	4.32	0.3
Wi(**D**)	$2.393\,38 \times 10$	$1.365\,07 \times 10^{-1}$	0.9625	1.17	1659.8
Wi(**RD**)	$1.826\,33 \times 10$	$1.063\,08$	0.8606	2.20	376.9
Wi(**CD**)	$2.699\,68 \times 10$	$7.921\,39 \times 10^{-2}$	0.8953	1.92	533.3
Wi(**RCD**)	$3.210\,30 \times 10$	$4.503\,12 \times 10^{-1}$	0.3875	3.98	23.3
Wi(**RW**)	$2.917\,61 \times 10$	$8.730\,40 \times 10^{-2}$	0.8487	2.28	339.9
$W_{e+o}(1,1)$	$2.393\,38 \times 10$	$1.365\,07 \times 10^{-1}$	0.9625	1.17	1659.8
$W_{e+o}(0.5,1)$	$2.353\,57 \times 10$	$1.788\,04 \times 10^{-1}$	0.9567	1.26	1427.0
$W_{e+o}(1,0.5)$	$2.331\,66 \times 10$	$1.780\,26 \times 10^{-1}$	0.9553	1.28	1379.3
$W_{e+o}(0.5,0.5)$	$2.212\,16 \times 10$	$2.631\,67 \times 10^{-1}$	0.9542	1.29	1342.6
$W_{e+o}(1.5,1)$	$2.528\,38 \times 10$	$8.740\,43 \times 10^{-2}$	0.9497	1.35	1213.4
$W_{e+o}(1.5,1.5)$	$2.593\,75 \times 10$	$6.481\,41 \times 10^{-2}$	0.9489	1.36	1194.3
$W_{e+o}(1,1.5)$	$2.557\,78 \times 10$	$8.647\,76 \times 10^{-2}$	0.9465	1.39	1136.7
$W_{e•o}(1,0.5)$	$2.930\,29 \times 10$	$5.108\,66 \times 10^{-3}$	0.9378	1.50	963.7
$W_{e+o}(1.5,0.5)$	$2.533\,17e \times 10$	$1.014\,19 \times 10^{-1}$	0.9371	1.51	951.7
$W_{e+o}(-0.5,1)$	$2.406\,06 \times 10$	$2.241\,23 \times 10^{-1}$	0.9364	1.52	940.6
$W_{e+o}(-0.5,0.5)$	$2.182\,75 \times 10$	$3.883\,55 \times 10^{-1}$	0.9355	1.53	924.6
$W_{e•o}(0.5,0.5)$	$2.880\,99 \times 10$	$9.518\,25 \times 10^{-3}$	0.9344	1.54	909.0
$W_{e+o}(0.5,1.5)$	$2.583\,17 \times 10$	$1.001\,63 \times 10^{-1}$	0.9332	1.55	889.6
$W_{e•o}(0.5,1)$	$2.948\,20 \times 10$	$5.259\,39 \times 10^{-3}$	0.9322	1.56	875.0
$W_{e+o}(1,-0.5)$	$2.348\,22 \times 10$	$2.190\,25 \times 10^{-1}$	0.9316	1.57	867.2

[a] The QSPR models have the general form $\Delta_{vap}H_{300} = a_0 + a_1$SD.

(p,q), followed by 4 $W_{e+o}(p,q)$ indices, all computed with positive p and q parameters. The best even/odd distance index, $W_{e•o}(2,1)$, with $r = 0.9087$, $s = 0.72$, and $F = 75.8$, surpasses all connectivity and Wiener-like indices; from this reference set of topological indices, only the first-order connectivity index $^0\chi$ gives comparable results, with $r = 0.8977$, $s = 0.76$, and $F = 66.4$. However, when modeling the size and shape effects upon alkane $\Delta_{vap}H_{300}$, the second-order connectivity index $^0\chi$ gives the best results ($r = 0.9785$, $s = 0.89$, and F = 2968.0), as one can see from Table 11. The top even/odd distance index is $W_{e+o}(1,1)$, with $r = 0.9625$, $s = 1.17$, and $F = 1659.8$; at a closer look one discovers that this is the classical Wiener index, **Wi(D)**.

Table 12. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with Two Independent Variables To Model the Vaporization Enthalpy at 300 K, $\Delta_{vap}H_{300}$ (kJ mol^{-1}), of 134 C_6–C_{10} Alkanes[a]

SD	a_0	a_1	a_2	r	s	F
$^0\chi$	7.323 09	1.020 54 × 10	−8.361 04	0.9866	0.71	2398.8
$^1\chi$	4.354 04	−1.386 29 × 10^{-1}	8.387 94	0.9785	0.89	1476.7
$^2\chi$	3.377 90	4.621 15	−2.054 51	0.9662	1.12	920.0
$^3\chi_p$	2.972 34	4.132 21	−1.233 30	0.9393	1.49	490.5
$^3\chi_c$	3.910 07	3.930 75	−1.703 79	0.9651	1.14	889.3
Wi(**D**)	2.087 19 × 10	5.435 94 × 10^{-1}	1.180 19 × 10^{-1}	0.9633	1.16	844.5
Wi(**RD**)	−1.619 98 × 10	9.941 51	−1.971 81	0.9755	0.95	1285.8
Wi(**CD**)	1.126 02 × 10	2.376 12	3.617 56 × 10^{-2}	0.9601	1.21	772.5
Wi(**RCD**)	2.305 69	4.380 92	−3.272 09 × 10^{-1}	0.9568	1.26	710.0
Wi(**RW**)	1.002 72 × 10	2.657 35	3.646 87 × 10^{-2}	0.9604	1.21	778.8
$W_{e+o}(-1.5,-2)$	−9.476 50	9.275 80	−2.718 83	0.9796	0.87	1560.1
SumE(−2)	−2.632 54	5.789 27	−4.132 28	0.9791	0.88	1518.4
$W_{e+o}(-2,-2)$	−8.786 35	9.627 58	−3.369 05	0.9788	0.89	1494.7
$W_{e+o}(-1,-1.5)$	−1.301 68 × 10	9.442 03	−2.077 66	0.9777	0.91	1417.0
$W_{e+o}(-1.5,-1.5)$	−1.092 61 × 10	9.323 12	−2.484 57	0.9775	0.91	1409.3
$W_{e\cdot o}(-2,-2)$	−1.178 55 × 10	6.636 02	−3.842 13 × 10^{-1}	0.9772	0.92	1384.9
SumE(−1.5)	−4.222 94	6.072 73	−2.977 12	0.9767	0.93	1358.7
$W_{e\cdot o}(-2,-1.5)$	−1.206 28 × 10	6.637 58	−3.416 26 × 10^{-1}	0.9767	0.93	1354.3
$W_{e+o}(-1,-2)$	−1.102 10 × 10	9.071 85	−2.105 54	0.9765	0.93	1347.4
$W_{o/e}(-2,-2)$	−1.332 52 × 10	4.296 69	3.789 75	0.9762	0.94	1327.8
$W_{e+o}(-1,-1)$	−1.619 99 × 10	9.941 55	−1.971 82	0.9755	0.95	1285.8
$W_{e\cdot o}(-2,-1)$	−1.265 26 × 10	6.671 86	−2.863 63 × 10^{-1}	0.9751	0.96	1264.7
$W_{e\cdot o}(-1.5,-2)$	−1.354 94 × 10	6.907 25	−2.724 72 × 10^{-1}	0.9748	0.97	1249.6
$W_{e\cdot o}(-1.5,-1.5)$	−1.388 25 × 10	6.917 55	−2.431 53 × 10^{-1}	0.9745	0.97	1236.9
$W_{o/e}(-2,-1.5)$	−1.151 71 × 10	4.137 64	3.366 28	0.9743	0.98	1224.0

[a] The QSPR models have the general form $\Delta_{vap}H_{300} = a_0 + a_1N + a_2$SD, where N is the number of carbon atoms.

Table 13. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with One Independent Variable To Model the Refractive Index at 25 °C, n_D^{25}, of 17 C_8 Alkanes[a]

SD	a_0	a_1	r	s	F
$^0\chi$	1.342 99	8.275 50 × 10^{-3}	0.2507	0.0051	1.0
$^1\chi$	1.396 39	2.614 48 × 10^{-4}	0.0070	0.0053	<0.1
$^2\chi$	1.406 14	−2.836 73 × 10^{-3}	0.2627	0.0051	1.1
$^3\chi_p$	1.376 56	1.160 95 × 10^{-2}	0.9758	0.0012	298.8
$^3\chi_c$	1.398 15	−9.920 08 × 10^{-4}	0.1074	0.0053	0.2
Wi(**D**)	1.431 27	−4.829 42 × 10^{-4}	0.5619	0.0044	6.9
Wi(**RD**)	1.315 84	5.523 82 × 10^{-3}	0.5205	0.0045	5.6
Wi(**CD**)	1.407 17	−1.021 59 × 10^{-4}	0.3906	0.0049	2.7
Wi(**RCD**)	1.390 86	6.269 05 × 10^{-4}	0.2470	0.0051	1.0
SumO(−2)	1.082 97	4.026 59 × 10^{-2}	0.9623	0.0014	187.6
SumO(−1.5)	1.192 07	2.434 99 × 10^{-2}	0.9386	0.0018	111.1
SumO(−1)	1.262 60	1.410 98 × 10^{-2}	0.8767	0.0026	49.8
$W_{e+o}(-2,-0.5)$	1.279 41	8.482 28 × 10^{-3}	0.8339	0.0029	34.2
$W_{e+o}(-1.5,-0.5)$	1.270 27	8.455 75 × 10^{-3}	0.8199	0.0030	30.8
$W_{e+o}(-2,-1)$	1.272 59	1.050 56 × 10^{-2}	0.7974	0.0032	26.2
$W_{e+o}(-1,-0.5)$	1.261 72	8.080 81 × 10	0.7548	0.0035	19.9
$W_{o/e}(-1,-1)$	1.371 26	9.418 36 × 10^{-2}	0.7393	0.0036	18.1
$W_{o/e}(0.5,-1.5)$	1.359 98	9.118 71 × 10^{-2}	0.7377	0.0036	17.9
$W_{o/e}(0.5,-1)$	1.363 14	7.364 08 × 10^{-2}	0.7364	0.0036	17.8
$W_{o/e}(1,-1.5)$	1.370 02	1.118 67 × 10^{-1}	0.7327	0.0036	17.4
SumO(−0.5)	1.315 58	7.062 27 × 10^{-3}	0.7323	0.0036	17.3
$W_{o/e}(1,-0.5)$	1.373 07	7.224 82 × 10^{-2}	0.7242	0.0037	16.5
$W_{o/e}(0.5,-2)$	1.358 00	1.037 28 × 10^{-1}	0.7227	0.0037	16.4
$W_{o/e}(1,-2)$	1.36922	1.244 15 × 10^{-1}	0.7181	0.0037	16.0

[a] The QSPR models have the general form $n_D^{25} = a_0 + a_1$SD.

Table 14. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with One Independent Variable To Model the Refractive Index at 25 °C, n_D^{25}, of 133 C_6–C_{10} Alkanes[a]

SD	a_0	a_1	r	s	F
N	1.307 95	1.103 60 × 10^{-2}	0.8751	0.0066	428.3
$^0\chi$	1.302 02	1.427 45 × 10^{-2}	0.9010	0.0059	564.8
$^1\chi$	1.320 23	2.126 64 × 10^{-2}	0.8028	0.0082	237.4
$^2\chi$	1.367 81	1.116 02 × 10^{-2}	0.5974	0.0110	72.7
$^3\chi_p$	1.363 84	2.043 87 × 10^{-2}	0.8859	0.0064	477.6
$^3\chi_c$	1.403 11	5.656 97 × 10^{-3}	0.2719	0.0132	10.5
Wi(**D**)	1.375 08	3.272 53 × 10^{-4}	0.7246	0.0094	144.8
Wi(**RD**)	1.341 97	3.597 59 × 10^{-3}	0.9205	0.0053	727.5
Wi(**CD**)	1.387 27	1.553 49 × 10^{-4}	0.5496	0.0114	56.7
Wi(**RCD**)	1.374 62	2.604 71 × 10^{-3}	0.7068	0.0097	130.8
Wi(**RW**)	1.393 66	1.505 62 × 10^{-4}	0.4578	0.0122	34.7
$W_{e+o}(-2,-1)$	1.337 52	4.844 29 × 10^{-3}	0.9322	0.0050	869.4
$W_{e+o}(-2,-1.5)$	1.332 63	5.813 58 × 10^{-3}	0.9303	0.0050	842.6
$W_{e+o}(-1.5,-1)$	1.339 11	4.302 06 × 10^{-3}	0.9291	0.0051	827.1
$W_{e+o}(-1.5,-1.5)$	1.335 44	5.028 60 × 10^{-3}	0.9249	0.0052	775.7
SumO(−1.5)	1.329 28	7.842 74 × 10^{-3}	0.9243	0.0052	768.0
$W_{e+o}(-2,-2)$	1.329 83	6.463 34 × 10^{-3}	0.9228	0.0053	751.3
SumO(−1)	1.337 07	6.104 95 × 10^{-3}	0.9227	0.0053	750.4
$W_{e+o}(-1,-1)$	1.341 97	3.597 59 × 10^{-3}	0.9205	0.0053	727.5
$W_{e+o}(-1.5,-0.5)$	1.345 25	3.314 27 × 10^{-3}	0.9202	0.0054	724.2
$W_{e+o}(-2,-0.5)$	1.344 96	3.609 04 × 10^{-3}	0.9195	0.0054	716.3
$W_{e+o}(-1.5,-2)$	1.333 52	5.492 85 × 10^{-3}	0.9168	0.0055	690.2
$W_{e+o}(-1,-0.5)$	1.346 43	2.893 90 × 10^{-3}	0.9167	0.0055	689.7
SumO(−2)	1.324 13	9.146 92 × 10^{-3}	0.9164	0.0055	686.4
$W_{e+o}(-1,-1.5)$	1.339 69	4.074 21 × 10^{-3}	0.9139	0.0056	664.3
$W_{e\cdot o}(-2,-1)$	1.371 78	1.030 28 × 10^{-3}	0.9132	0.0056	657.9

[a] The QSPR models have the general form $n_D^{25} = a_0 + a_1$SD.

Therefore, for the alkane vaporization enthalpy of the whole set of 134 molecules, **Wi(D)** is superior to all even/odd distance descriptors investigated in this paper; this is not surprising, since we cannot expect that a group of structurally related indices will give the best QSAR in all instances. A similar situation is detected in Table 12, where we present the biparametric $\Delta_{vap}H_{300}$ QSPR equations for the entire set of 134 alkanes. The best equation is obtained with $^0\chi$ (r = 0.9866, s = 0.71, and F = 2398.8), while the second place is occupied by $W_{e+o}(-1.5,-2)$, with r = 0.9796, s = 0.87, and F = 1560.1. The next descriptor is SumE(−2); we have to mention that from the whole set of 12 QSPR experiments

Table 15. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with Two Independent Variables To Model the Refractive Index at 25 °C, n_D^{25}, of 133 C_6–C_{10} Alkanes[a]

SD	a_0	a_1	a_2	r	s	F
$^0\chi$	1.301 77	$-3.034\,41 \times 10^{-3}$	$1.801\,51 \times 10^{-2}$	0.9022	0.0059	284.3
$^1\chi$	1.308 06	$1.558\,56 \times 10^{-2}$	$-1.000\,51 \times 10^{-2}$	0.8822	0.0065	228.2
$^2\chi$	1.308 01	$1.097\,94 \times 10^{-2}$	$1.236\,32 \times 10^{-4}$	0.8751	0.0067	212.6
$^3\chi_p$	1.320 96	$6.551\,60 \times 10^{-3}$	$1.268\,88 \times 10^{-2}$	0.9705	0.0033	1051.8
$^3\chi_c$	1.308 33	$1.084\,27 \times 10^{-2}$	$1.313\,98 \times 10^{-3}$	0.8772	0.0066	217.0
Wi(**D**)	1.230 50	$2.575\,45 \times 10^{-2}$	$-5.525\,42 \times 10^{-4}$	0.9490	0.0043	588.6
Wi(**RD**)	1.381 61	$-1.138\,84 \times 10^{-2}$	$7.067\,58 \times 10^{-3}$	0.9352	0.0049	453.0
Wi(**CD**)	1.282 01	$1.593\,88 \times 10^{-2}$	$-1.351\,40 \times 10^{-4}$	0.9183	0.0054	349.6
Wi(**RCD**)	1.314 08	$8.956\,42 \times 10^{-3}$	$9.770\,47 \times 10^{-4}$	0.8994	0.0060	275.1
Wi(**RW**)	1.286 78	$1.485\,83 \times 10^{-2}$	$-1.351\,63 \times 10^{-4}$	0.9181	0.0054	348.6
SumO(−2)	1.386 86	$-3.369\,57 \times 10^{-2}$	$3.564\,04 \times 10^{-2}$	0.9663	0.0035	917.2
SumO(−1.5)	1.376 79	$-1.978\,96 \times 10^{-2}$	$2.099\,60 \times 10^{-2}$	0.9559	0.0040	689.1
$W_{e+o}(-2,-1)$	1.379 67	$-1.320\,02 \times 10^{-2}$	$1.018\,00 \times 10^{-2}$	0.9541	0.0041	659.8
$W_{e+o}(1.5,1.5)$	1.253 68	$2.078\,28 \times 10^{-2}$	$-1.864\,32 \times 10^{-4}$	0.9497	0.0043	597.7
$W_{e+o}(1,1)$	1.230 50	$2.575\,45 \times 10^{-2}$	$-5.525\,42 \times 10^{-4}$	0.9490	0.0043	588.6
$W_{e+o}(-2,-1.5)$	1.365 64	$-1.189\,19 \times 10^{-2}$	$1.159\,00 \times 10^{-2}$	0.9488	0.0043	586.3
$W_{e+o}(2,2)$	1.266 23	$1.821\,33 \times 10^{-2}$	$-6.752\,21 \times 10^{-5}$	0.9487	0.0043	585.0
$W_{e+o}(-1.5,-1)$	1.380 36	$-1.248\,91 \times 10^{-2}$	$8.801\,75 \times 10^{-3}$	0.9485	0.0044	582.3
$W_{e+o}(1.5,2)$	1.266 78	$1.819\,30 \times 10^{-2}$	$-9.009\,90 \times 10^{-5}$	0.9449	0.0045	541.2
$W_{e+o}(1.5,1)$	1.251 27	$2.145\,23 \times 10^{-2}$	$-2.638\,80 \times 10^{-4}$	0.9439	0.0045	530.8
$W_{e+o}(2,1.5)$	1.264 83	$1.858\,63 \times 10^{-2}$	$-9.540\,16 \times 10^{-5}$	0.9437	0.0045	529.2
$W_{e+o}(1,1.5)$	1.255 32	$2.062\,74 \times 10^{-2}$	$-2.431\,60 \times 10^{-4}$	0.9420	0.0046	512.0
$W_{e+o}(1,0.5)$	1.227 29	$2.684\,35 \times 10^{-2}$	$-7.719\,35 \times 10^{-4}$	0.9403	0.0047	496.6
$W_{e+o}(0.5,0.5)$	1.179 87	$3.727\,36 \times 10^{-2}$	$-1.848\,78 \times 10^{-3}$	0.9402	0.0047	495.5
$W_{e\cdot o}(1,2)$	1.267 61	$1.690\,32 \times 10^{-2}$	$-1.338\,10 \times 10^{-6}$	0.9398	0.0047	491.9

[a] The QSPR models have the general form $n_D^{25} = a_0 + a_1N + a_2$SD, where N is the number of carbon atoms.

Table 16. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with One Independent Variable To Model the Alkane Density at 25 °C, ρ (kg m^{-3}), of 17 C_8 Alkanes[a]

SD	a_0	a_1	r	s	F
$^0\chi$	$5.707\,55 \times 10^2$	$2.044\,94 \times 10$	0.2820	11.18	1.3
$^1\chi$	$7.112\,88 \times 10^2$	−1.694 52	0.0206	11.65	<0.1
$^2\chi$	$7.226\,05 \times 10^2$	−5.655 71	0.2384	11.32	0.9
$^3\chi_p$	$6.592\,91 \times 10^2$	$2.556\,47 \times 10$	0.9780	2.43	329.6
$^3\chi_c$	$7.064\,18 \times 10^2$	−1.674 59	0.0825	11.61	0.1
Wi(**D**)	$7.841\,20 \times 10^2$	−1.125 48	0.5960	9.36	8.3
Wi(**RD**)	$5.153\,72 \times 10^2$	$1.285\,62 \times 10$	0.5514	9.72	6.6
Wi(**CD**)	$7.288\,89 \times 10^2$	$-2.478\,00 \times 10^{-1}$	0.4313	10.51	3.4
Wi(**RCD**)	$6.886\,42 \times 10^2$	1.586 93	0.2845	11.17	1.3
SumO(−2)	$1.165\,53 \times 10$	$8.881\,43 \times 10$	0.9660	3.01	209.5
SumO(−1.5)	$2.539\,85 \times 10^2$	$5.350\,63 \times 10$	0.9388	4.01	111.3
SumO(−1)	$4.108\,88 \times 10^2$	$3.080\,58 \times 10$	0.8712	5.72	47.2
$W_{e+o}(-2,-0.5)$	$4.449\,67 \times 10^2$	$1.870\,74 \times 10$	0.8371	6.37	35.1
$W_{e+o}(-1.5,-0.5)$	$4.223\,94 \times 10^2$	$1.880\,98 \times 10$	0.8301	6.50	33.2
$W_{e+o}(-2,-1)$	$4.247\,05 \times 10^2$	$2.360\,87 \times 10$	0.8156	6.74	29.8
$W_{e+o}(-1,-0.5)$	$3.993\,10 \times 10^2$	$1.821\,77 \times 10$	0.7745	7.37	22.5
$W_{o/e}(1,-1)$	$6.471\,54 \times 10^2$	$2.091\,08 \times 10^2$	0.7471	7.74	18.9
$W_{o/e}(1,-1.5)$	$6.442\,74 \times 10^2$	$2.488\,64 \times 10^2$	0.7418	7.81	18.4
$W_{o/e}(0.5,-1.5)$	$6.231\,11 \times 10^2$	$2.000\,02 \times 10^2$	0.7364	7.88	17.8
$W_{o/e}(0.5,-1)$	$6.301\,51 \times 10^2$	$1.612\,72 \times 10^2$	0.7340	7.91	17.5
$W_{o/e}(1,-0.5)$	$6.513\,41 \times 10^2$	$1.598\,71 \times 10^2$	0.7293	7.97	17.0
$W_{o/e}(1,-2)$	$6.424\,22 \times 10^2$	$2.771\,13 \times 10^2$	0.7280	7.99	16.9
$W_{o/e}(1.5,-1)$	$6.624\,12 \times 10^2$	$2.660\,28 \times 10^2$	0.7254	8.02	16.7
$W_{o/e}(0.5,-2)$	$6.187\,60 \times 10^2$	$2.275\,56 \times 10^2$	0.7216	8.07	16.3

[a] The QSPR models have the general form $\rho = a_0 + a_1$SD.

made for the 6 alkane properties, this is the single case when the sum of even distances SumE(p) gives better results than the sum of even distances SumO(q). Additional tests are needed, including more diverse organic compounds, to determine if this results has a broader significance.

Refractive Index. The first experiment for the alkane refractive index QSPR was made for 17 from the 18 octane isomers (the experimental value for 2,2,3,3-tetramethylbutane is missing); the results from Table 13 indicate that the "classical" indices perform badly, with the notable exception of $^3\chi_p$, with $r = 0.9758$, $s = 0.0012$, and $F = 298.8$. The connectivity index $^3\chi_p$ represents the weighted contribution of butane-like subgraphs and is a measure of molecular branching combined with some size contribution, due to the summation of the contributions of all linear subgraphs with four carbon atoms. The second best index is the sum of even distances SumO(−2), with $r = 0.9623$, $s = 0.0014$, and $F = 187.6$. In fact, all four SumO(q) indices with negative

Table 17. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with One Independent Variable To Model the Alkane Density at 25 °C, ρ (kg m^{-3}), of 133 C_6–C_{10} Alkanes[a]

SD	a_0	a_1	r	s	F
N	$5.360\,27 \times 10^2$	$2.083\,49 \times 10$	0.8545	13.75	354.4
$^0\chi$	$5.245\,26 \times 10^2$	$2.698\,82 \times 10$	0.8810	12.52	454.2
$^1\chi$	$5.583\,54 \times 10^2$	$4.035\,40 \times 10$	0.7879	16.30	214.4
$^2\chi$	$6.519\,08 \times 10^2$	$2.029\,18 \times 10$	0.5618	21.90	60.4
$^3\chi_p$	$6.369\,93 \times 10^2$	$4.064\,16 \times 10$	0.9110	10.91	639.6
$^3\chi_c$	$7.164\,14 \times 10^2$	9.974 80	0.2479	25.64	8.6
Wi(**D**)	$6.640\,45 \times 10^2$	$6.054\,36 \times 10^{-1}$	0.6933	19.07	121.3
Wi(**RD**)	$5.994\,59 \times 10^2$	6.834 62	0.9045	11.29	589.2
Wi(**CD**)	$6.872\,48 \times 10^2$	$2.827\,63 \times 10^{-1}$	0.5174	22.65	47.9
Wi(**RCD**)	$6.604\,84 \times 10^2$	5.023 25	0.7050	18.77	129.5
Wi(**RW**)	$6.992\,83 \times 10^2$	$2.701\,79 \times 10^{-1}$	0.4249	23.96	28.9
$W_{e+o}(-2,-1)$	$5.905\,44 \times 10^2$	9.234 22	0.9191	10.43	712.6
$W_{e+o}(-2,-1.5)$	$5.814\,24 \times 10^2$	$1.106\,59 \times 10$	0.9158	10.63	681.5
$W_{e+o}(-1.5,-1)$	$5.937\,26 \times 10^2$	8.190 49	0.9149	10.69	672.7
SumO(−1.5)	$5.747\,37 \times 10^2$	$1.495\,89 \times 10$	0.9118	10.87	645.7
SumO(−1)	$5.893\,97 \times 10^2$	$1.166\,07 \times 10$	0.9115	10.89	643.4
$W_{e+o}(-1.5,-1.5)$	$5.869\,53 \times 10^2$	9.559 54	0.9094	11.01	626.4
$W_{e+o}(-2,-2)$	$5.763\,75 \times 10^2$	$1.227\,91 \times 10$	0.9067	11.16	605.4
$W_{e+o}(-2,-0.5)$	$6.047\,45 \times 10^2$	6.878 20	0.9063	11.19	602.4
$W_{e+o}(-1.5,-0.5)$	$6.054\,06 \times 10^2$	6.310 40	0.9062	11.19	601.7
$W_{e+o}(-1,-1)$	$5.994\,59 \times 10^2$	6.834 62	0.9045	11.29	589.2
SumO(−2)	$5.653\,04 \times 10^2$	$1.740\,50 \times 10$	0.9018	11.44	570.7
$W_{e+o}(-1,-0.5)$	$6.078\,72 \times 10^2$	5.500 39	0.9012	11.47	566.2
$W_{e+o}(-1.5-,2)$	$5.835\,61 \times 10^2$	$1.042\,33 \times 10$	0.8998	11.55	556.9
$W_{e\cdot o}(-2,-1)$	$6.560\,99 \times 10^2$	1.956 69	0.8970	11.70	539.5
$W_{e+o}(-1,-1.5)$	$5.953\,20 \times 10^2$	7.728 07	0.8966	11.72	537.0

[a] The QSPR models have the general form $\rho = a_0 + a_1$SD.

Table 18. Structural Descriptors SD, Coefficients, and Statistical Indices for Linear Regression Equations with Two Independent Variables To Model the Alkane Density at 25 °C, ρ (kg m^{-3}), of 133 C_6–C_{10} Alkanes[a]

SD	a_0	a_1	a_2	r	s	F
$^0\chi$	$5.239\,87 \times 10^2$	−6.554 18	$3.506\,76 \times 10$	0.8825	12.50	228.9
$^1\chi$	$5.362\,11 \times 10^2$	$2.835\,85 \times 10$	$-1.654\,54 \times 10$	0.8598	13.57	184.3
$^2\chi$	$5.354\,25 \times 10^2$	$2.138\,80 \times 10$	−1.207 54	0.8548	13.79	176.4
$^3\chi_p$	$5.641\,98 \times 10^2$	$1.112\,04 \times 10$	$2.748\,72 \times 10$	0.9752	5.88	1262.5
$^3\chi_c$	$5.365\,27 \times 10^2$	$2.058\,01 \times 10$	1.731 54	0.8555	13.76	177.4
Wi(**D**)	$3.705\,13 \times 10^2$	$5.228\,59 \times 10$	−1.180 69	0.9459	8.62	552.3
Wi(**RD**)	$6.884\,74 \times 10^2$	$-2.557\,88 \times 10$	$1.462\,83 \times 10$	0.9245	10.13	382.3
Wi(**CD**)	$4.810\,89 \times 10^2$	$3.121\,72 \times 10$	$-2.861\,78 \times 10^{-1}$	0.9072	11.18	302.2
Wi(**RCD**)	$5.486\,73 \times 10^2$	$1.654\,15 \times 10$	2.017 13	0.8827	12.48	229.4
Wi(**RW**)	$4.912\,26 \times 10^2$	$2.892\,28 \times 10$	$-2.860\,08 \times 10^{-1}$	0.9069	11.20	301.0
SumO(−2)	$7.079\,34 \times 10^2$	$-7.662\,01 \times 10$	$7.764\,81 \times 10$	0.9713	6.32	1084.4
SumO(−1.5)	$6.866\,76 \times 10^2$	$-4.662\,92 \times 10$	$4.595\,11 \times 10$	0.9590	7.53	744.9
$W_{e+o}(-2,-1)$	$6.880\,17 \times 10^2$	$-3.052\,88 \times 10$	$2.157\,44 \times 10$	0.9507	8.24	610.2
$W_{e+o}(1.5,1.5)$	$4.199\,64 \times 10^2$	$4.167\,92 \times 10$	$-3.987\,02 \times 10^{-1}$	0.9469	8.54	563.9
$W_{e+o}(2,2)$	$4.466\,55 \times 10^2$	$3.620\,88 \times 10$	$-1.446\,33 \times 10^{-1}$	0.9459	8.62	552.9
$W_{e+o}(1,1)$	$3.705\,13 \times 10^2$	$5.228\,59 \times 10$	−1.180 69	0.9459	8.62	552.3
$W_{e+o}(-1.5,-1)$	$6.879\,86 \times 10^2$	$-2.853\,43 \times 10$	$1.847\,11 \times 10$	0.9422	8.90	513.9
$W_{e+o}(-2,-1.5)$	$6.564\,62 \times 10^2$	$-2.703\,31 \times 10$	$2.419\,71 \times 10$	0.9417	8.94	509.2
$W_{e+o}(1.5,1)$	$4.134\,37 \times 10^2$	$4.336\,15 \times 10$	$-5.706\,77 \times 10^{-1}$	0.9416	8.95	508.3
$W_{e+o}(2,1.5)$	$4.427\,60 \times 10^2$	$3.716\,43 \times 10$	$-2.063\,30 \times 10^{-1}$	0.9414	8.96	506.5
$W_{e+o}(1.5,2)$	$4.486\,96 \times 10^2$	$3.601\,46 \times 10$	$-1.910\,99 \times 10^{-1}$	0.9396	9.09	490.1
$W_{e+o}(1,0.5)$	$3.609\,41 \times 10^2$	$5.514\,67 \times 10$	−1.675 57	0.9378	9.23	474.0
$W_{e+o}(1,1.5)$	$4.247\,04 \times 10^2$	$4.111\,99 \times 10$	$-5.142\,65 \times 10^{-1}$	0.9357	9.37	457.3
$W_{e+o}(0.5,0.5)$	$2.614\,95 \times 10^2$	$7.707\,13 \times 10$	−3.962 60	0.9356	9.38	456.7
SumO(−1)	$6.716\,20 \times 10^2$	$-2.661\,14 \times 10$	$2.536\,29 \times 10$	0.9352	9.41	453.5

[a] The QSPR models have the general form $\rho = a_0 + a_1N + a_2$SD, where N is the number of carbon atoms.

values for the parameter q are present in Table 13, showing that better correlations are obtained if longer graph distances have a lower weight. The second QSPR experiment for n_D^{25} was performed for the whole group of 133 alkanes (Tables 14 and 15). Overall, the distance sum indices $W_{e+o}(p,q)$ with negative p and q parameters give the best QSPR models; three SumO indices are present in the top 15 QSPR models, namely, SumO(−1.5), SumO(−1), and SumO(−2). The first position is occupied by $W_{e+o}(-2,-1)$, with $r = 0.9322$, $s = 0.0050$, and $F = 869.4$, while from the reference set of indices, only **Wi(RD)** has comparable statistical indices ($r = 0.9205$, $s = 0.0053$, and $F = 727.5$). In the second QSPR experiment for the alkane refractive index, the combination between N and $^3\chi_p$ gives the best results, with $r = 0.9705$, s

= 0.0033, and $F = 1051.8$, while the weighted sum of odd distances SumO(−2) comes in second place, with $r = 0.9663$, $s = 0.0035$, and $F = 917.2$. Although not as good as the connectivity index $^3\chi_p$, the even/odd distance descriptors are highly relevant for the modeling of the alkane refractive index.

Density. In Table 16 we present the density QSPR monoparametric models obtained for 17 octane isomers (2,2,3,3-tetramethylbutane was not considered in correlations). A comparison between the results reported in Tables 13 and 16 reveals a significant similarity between the QSPR models for octane refractive index and density. Indeed, from the reference set of indices, only $^3\chi_p$ gives good results, with $r = 0.9780$, $s = 2.43$, and $F = 329.6$. This connectivity index is followed by SumO(−2) ($r = 0.9660$, $s = 3.01$, and $F = 209.5$), SumO(−1.5), and SumO(−1). When the whole set of 133 alkanes is used to develop monoparametric QSPR models, even/odd distance descriptors are clearly superior to the reference set of indices, as can be seen from Table 17. The even/odd distance sum index $W_{e+o}(-2,-1)$ is the first, with $r = 0.9191$, $s = 10.43$, and $F = 712.6$. In the top 15 even/odd distance descriptors one finds 11 indices $W_{e+o}(p,q)$, 3 indices SumO(q), and a single $W_{e\text{-}o}(p,q)$ index, all of them being computed with negative p and q parameters. From the set of "classical" indices, $^3\chi_p$ is the best, with $r = 0.9110$, $s = 10.91$, and $F = 639.6$. This situation changes when passing to biparametric QSPR equations (Table 18), when the pair of descriptors N and $^3\chi_p$ provides the best combination, with $r = 0.9752$, $s = 5.88$, and $F = 1262.5$. The second place is occupied by the pair N and SumO(−2), with $r = 0.9713$, $s = 6.32$, and $F = 1084.4$. Good QSPR models for the alkane density are also obtained with SumO(−1.5), followed by a group of $W_{e+o}(p,q)$ indices. Compared with the Wiener-like indices, in all density QSPR models the even/odd distance descriptors give superior results. Even if for octanes and in biparametric QSPR models the connectivity index $^3\chi_p$ comes first, the novel even/odd distance descriptors are very close and can be interesting candidates in multiparametric models.

CONCLUDING REMARKS

Topological indices derived from the molecular graph of organic compounds represent valuable structural descriptors that can be used with success in developing QSPR and QSAR models. The use of molecular graph descriptors in QSAR/QSPR models is intended to complement other classes of structural descriptors, such as fingerprints, hydrophobicity, counts of various structural features, geometrical, electrostatic, and quantum descriptors. Two classes of graph descriptors are extensively used in QSAR/QSPR models, namely, the connectivity[1,2] and distance-related descriptors. The studies presented in this paper were stimulated by the possibility of improving the correlational power of Wiener-like indices by separating the interatomic distances into two groups, i.e., even and odd graph distances, and summing them separately into even/odd distance indices SumE(p) and SumO(q). These two graph invariants are combined into a series of new graph descriptors that measure the molecular size and shape, namely, $W_{e+o}(p,q)$, $W_{e/o}(p,q)$, $W_{o/e}(p,q)$, and $W_{e\text{-}o}(p,q)$. Structural descriptors computed with these novel indices were used to develop QSPR models for six alkane properties: normal boiling temperature, molar heat capacity, standard Gibbs energy of formation, vaporization enthalpy, refractive index, and density. To estimate the QSPR value of the novel indices, we have computed similar structure−property models for 5 connectivity and 4 Wiener-like indices.

This comparative study clearly demonstrates that the concept of splitting the graph distances into even/odd categories is often successful, giving structural descriptors with notably improved correlational power. It is important to point out that, in the majority of QSPR models investigated in this paper, the best results are obtained with even/odd distance indices SumO(q), $W_{e+o}(p,q)$, $W_{o/e}(p,q)$, and $W_{e\text{-}o}(p,q)$ computed with negative values for the parameters p and q. The importance of negative power coefficients in the design of topological indices with an improved correlational power was also emphasized in the definitions of several molecular matrices and graph descriptors, such as the reciprocal distance matrix **RD**,[27−31] the distance−valency matrix **Dval**,[34] the reciprocal complementary distance matrix **RCD**,[35] the connectivity index χ,[67] the Ivanciuc−Balaban operator **IB**,[23] information−theoretical indices based on vertex distances U, V, X, and Y [55−57] and the corresponding graph operators **U**(**M**), **V**(**M**), **X**(**M**), and **Y**(**M**),[58,59] and regressive distance descriptors.[68,69] We have also observed that in a large number of QSPR models the sum of odd distances SumO(q) gives better results than the sum of even distances SumE(p); QSPR and QSAR tests with more diverse organic compounds are needed to determine if these results have a broader significance. An interesting research direction would be the extension of these even/odd distance indices to vertex- and edge-weighted molecular graphs, representing organic compounds with heteroatoms and multiple bonds. This task should be aided by several weighting schemes which are already used for structural descriptors based on the distance matrix.[11,20−23]

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