

GRAPH DISSECTION REVISITED. APPLICATION TO SMALLER ALKANES**Milan Randić,^{a,b} Xiaofeng Guo,^{a,c} and Paula Calkins^a**^a Department of Mathematics and Computer Science, Drake University, Des Moines, Iowa 50311, USA;^b National Institute of Chemistry, Hajdrihova 19, P. O. Box 3430, Ljubljana, Slovenia^c Institute of Mathematics and Physics, Xinjiang University, Wulumuqi Xinjiang 830046, P. R. China*Received 02-11-1998***Abstract**

Dissection of graphs was outlined twenty years ago as a scheme to arrive at an integer characterization of graphs. The approach, which raises some mathematical questions as well as it offers novel structural descriptors of potential interest in structure-property studies, was apparently overlooked. In this contribution we have re-examined graph dissection, we corrected some errors in the earlier publications, and illustrate use of novel descriptors derived through the dissection process in structure-property correlation for selected properties of octane isomers.

Introduction

With hundreds of topological indices one would expect that most molecules could be well characterized and their physicochemical properties correlated with the available descriptors. However, a number of properties even of alkanes, which are the simplest structures to consider in view that they lack the complications caused by the presence of heteroatoms, still can not be well described with available descriptors. For example, this is the case with critical temperature, critical pressure and critical volume. In addition the steric parameters of octanes also cannot be well correlated with most of the available molecular topological indices. Hence, the search for novel molecular descriptors continues.

Recently a number of novel molecular descriptors were outlined. Let us mention few: The novel shape descriptors represented as the ratio of the count of paths and walks of the same length,^{1, 2} the novel chirality index for planar structures (e. g., planar benzenoid hydrocarbons),³ a "missing" descriptor p_3^* which count the paths of length three for heteroatoms.⁴ We would like to add to this list the descriptors a, b which count the atom and the bond components in a successive dissection of graphs, outlined twenty

years ago by one of the present authors.^{5,6} As we will see the novel parameters a , and b , which are integers, are on one side very sensitive to molecular branching and on the other hand appears to be unique, at least for smaller trees. Hence, their mathematical properties may be of interest, particularly if the high discrimination among isomers is shown to hold for larger structures. Here, we will be primarily interested in use of the novel descriptors a , b in structure-property relation, which is the sole and the ultimate criterion for a justification of introducing novel topological indices.

Dissection of Graphs

Dissection of graphs was defined as a stepwise process in which one removes one vertex at a time from the graph considered and continues to do so on all subgraphs, which are neither isolated vertices nor isolated bonds. Formally we have Definition: Dissection (a , b) of a graph G is collection of subgraphs A and B obtained by erasing one vertex at a time from a graph G and all its so obtained subgraphs G^* generated from G which neither represent isolated vertices A nor isolated bonds B .

In Fig.1 we illustrate the steps involved in dissection process for n -butane. First we erase the four vertices, one at a time. This generated four subgraphs shown in the middle part of Fig. 1. The derived subgraphs are, in fact, the Ulam's subgraphs of n -butane. Ulam's subgraphs arise in the famous, still unresolved, problem of the graph reconstruction.^{7, 8} In the next step we continue by dissection of the two propane fragments, which gives as fragments only isolated vertices and isolated edges signaling the end of step-wise dissection. By counting all isolated vertices (atoms) and isolated edges (bonds) we obtain the two parameters a and b , respectively.

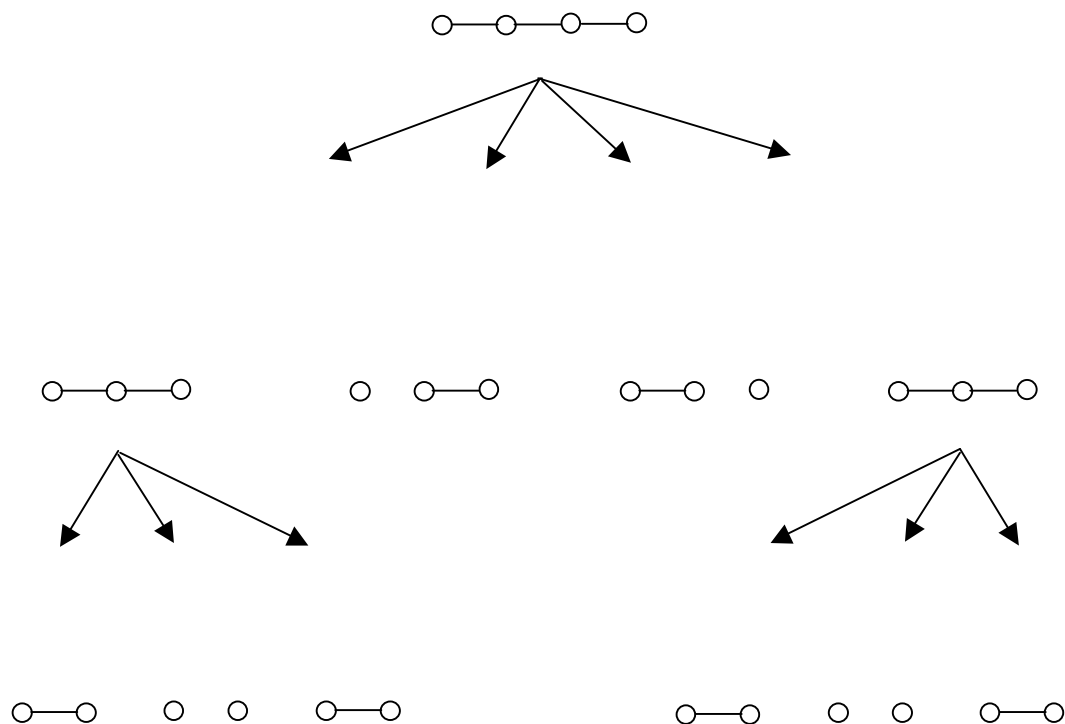


Fig. 1 Dissection of n-butane: $6a + 6b$

Dissection of n-pentane isomers is illustrated in Fig. 2. After the first step we obtained as components n-butane, isobutane, and propane fragments. In the next step we dissected graphs of propane, butane, and isobutane, which as one can easily verify give: $(2a + 2b)$, $(6a + 6b)$ and $(9a + 6b)$, respectively. With this information we obtain for the three pentane isomers of Fig.2 as the overall decomposition: $(18a + 18b)$, $(26a + 21b)$ and $(40a + 24b)$ respectively.

In Table 1 we give the dissection parameters a , b for the five isomers of hexane, the nine isomers of heptane and the 18 isomers of octane. The a , b parameters for smaller alkanes were reported in ref. (5), but because of the numerical errors for 2,2-dimethylbutane, 2,3-dimethylbutane and 2-methylhexane the results for more branched heptanes and octanes were also in error so we give here the revised corrected values. The entries in Table 1 were ordered by increasing values of the parameters a , b . As we see

the both parameters increase with molecular branching. Observe also that the range of the values assumed by a and b increases with the size of molecules. On this base alone one may expect few degeneracy, if any, which if shown to persist will make (a, b) parameters of interest in graph isomorphism problem.⁹⁻¹¹

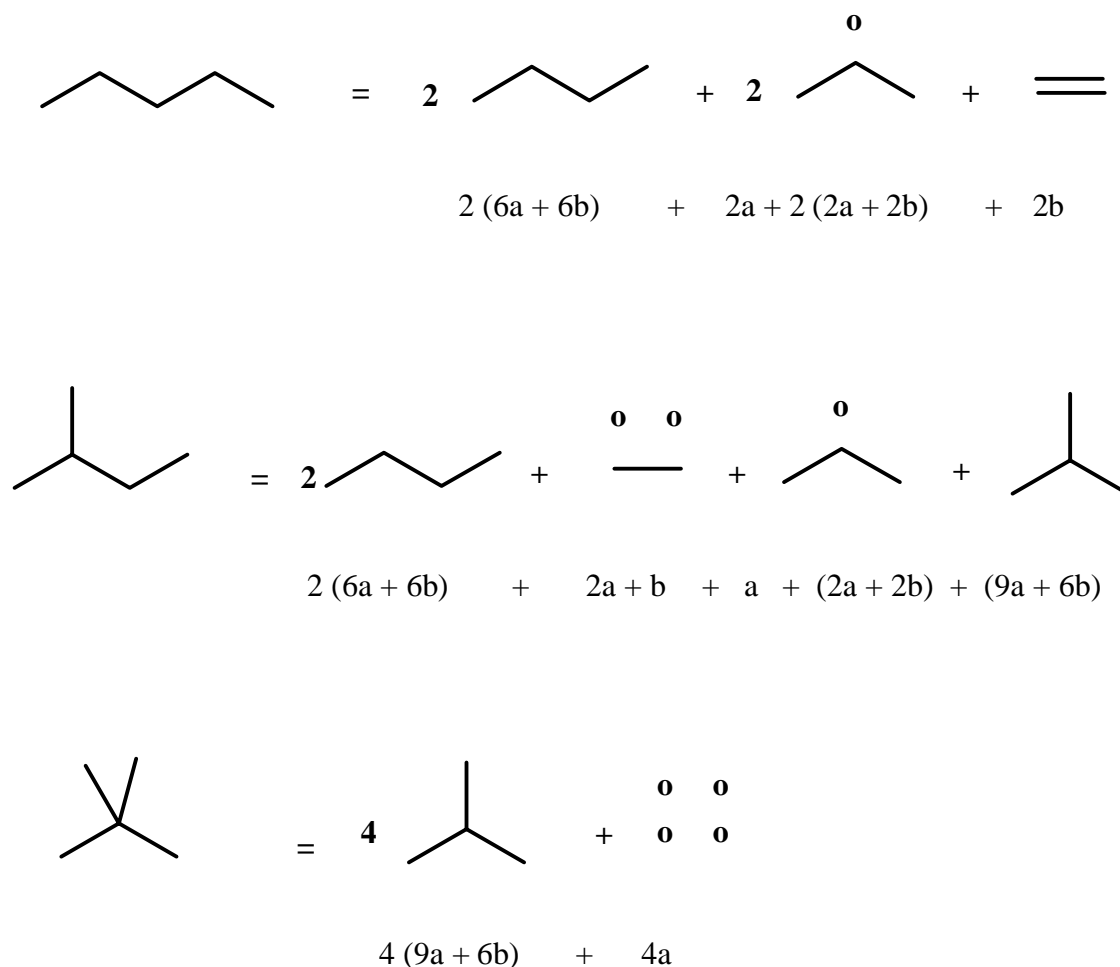


Fig. 2 Dissection of pentane, 2-methylbutane and 2,2-dimethylpropane

There are several graph invariants of a very high-resolution power¹²⁻¹⁶ that may be of interest for graph isomorphism testing. The present invariants (a, b) are the first

integers that may show similar properties and as such deserve further attention in that respect -- which is not the subject of the present study.

Table I: The dissection parameters a , b for the smaller alkanes

Hexanes		Octanes	
n-hexane	54 a + 54 b	n-octane	486 a + 486 b
2-methyl	78 a + 68 b	2-methyl	702 a + 662 b
3-methyl	85 a + 74 b	3-methyl	850 a + 786 b
2,3-dimethyl	112 a + 88 b	4-methyl	905 a + 830 b
2,2-dimethyl	131 a + 94 b	2,5-dimethyl	1014 a + 914 b
		3-ethyl	1072 a + 974 b
Heptanes		2, 4-dimethyl	1241 a + 1096 b
n-heptane	162 a + 162 b	2, 2-dimethyl	1313 a + 1099 b
2-methyl	234 a + 214 b	2, 3-dimethyl	1337 a + 1167 b
3-methyl	272 a + 245 b	3, 4-dimethyl	1520 a + 1314 b
3-ethyl	312 a + 279 b	2-methyl-3-ethyl	1594 a + 1378 b
2, 4-dimethyl	338 a + 288 b	3, 3-dimethyl	1663 a + 1360 b
2, 3-dimethyl	395 a + 331 b	2, 2, 4-trimethyl	1917 a + 1550 b
2, 2-dimethyl	419 a + 324 b	3-methyl-3-ethyl	1948 a + 1581 b
3, 3-dimethyl	459 a + 359 b	2, 3, 4-trimethyl	1979 a + 1658 b
2, 2, 3-trimethyl	614 a + 460 b	2, 2, 3-trimethyl	2368 a + 1884 b
		2, 3, 3-trimethyl	2535 a + 1945 b
		2,2,3,3; tetramethyl	3708 a + 2772 b

Use of the Dissection Parameters a , b for QSAR

The importance of topological indices and other mathematical invariants of a chemical structural in QSAR rest solely on their use in structure-property and structure-activity studies. Topological indices may have additional use for detection of structural similarity / dissimilarity,^{17,18} for characterization of molecular branching,¹⁹⁻²⁶ cyclicality,²⁷⁻²⁹ molecular complexity,³⁰⁻³³ graph density,³⁴ the degree of convexity,³⁵ molecular,^{36, 37} the degree of folding for a long chain structure,³⁸⁻⁴⁰ etc. Finally, they may be of interest in chemical documentation, including use in the isomorphism and the automorphism problems. The justification for extending study of mathematical properties of such indices, for which apparently some practitioners in the field do not give sufficient attention, follows from their use. If an index outperforms other indices, or combinations of other indices in a correlation of a particular property, it is of interest to investigate its property and in an effort to identify the critical structural elements that make the index successful. Hence, we have to postpone mathematical study of the dissection parameters till we can demonstrate its use in structure-property-activity studies.

From Table 1 it is not immediately clear whether there is some regularity for the parameters a , b , except that they increase with molecular branching. It is also not apparent that such list of numbers has promise in structure-property studies. One way to find out is to test the new descriptors against a number of available molecular properties. However, it is possible in advance to assert whether these numbers, and for that matter any list of numbers associated with smaller alkanes, have promise in QSAR or not. All that is needed is to consult the "Periodic Table for Alkane Isomers."⁴¹⁻⁴³

In Table 2 we reproduce the "Periodic Table for Octane Isomers," which is derived from partial ordering of isomers based on the count of paths of length two and paths of length three, on which many physicochemical properties of alkanes depend. It was shown^{25, 41-43} that many properties as well as the values for many descriptors show a regular variation when their values for isomers are substituted in the corresponding site in the table. In Table 3 we show the variation of the parameter a obtained by dissection of octane isomers within the "Periodic Table." As we see the values increase from the top to the bottom and from the left to the right, with the only a minor numerical exception for

2, 3, 4-trimethylpentane and 3-methyl-3-ethylpentane. The values for 3-methylheptane and 4-methylheptane, which belong to the same cell of the periodic table, and the values for 2-methyl-3-ethylpentane and 3, 4-dimethylhexane which belong to another single cell, as we see from Table 3, differ little. This gives further support to the observed regular variation of the dissection parameters within the table.

Table 2 Periodic table for octane isomers

n-8				
2-methyl	3-methyl 4-methyl	3-ethyl		
2,5-dimethyl	2,4-dimethyl	2,3-dimethyl	3,4-dimethyl 2-methyl-3-ethyl	
2,2-dimethyl		3,3-dimethyl	2,3,4-trimethyl	3-methyl-3-ethyl
2,2,4-trimethyl			2,2,3-trimethyl	2,3,3-trimethyl
				2,2,3,3-tetramethyl

Table 3 Periodic table for octane isomers with inscribed dissection parameter a

486				
	850			
702	905	1072		
			1520	
1014	1241	1337	1594	
1313		1663	1979	1948
1917			2368	2535
				3708

We tested the parameters (a, b) against several physicochemical properties of octanes. The results are summarized in Table 4 for properties associated with the correlation coefficient close to 0.9000 or higher.

Table 4 Correlations of properties of octanes with descriptors (a, b)

Property	r (a, b)	s (a, b)	F (a, b)	r (a)	*see text
Steric factor	0.9861	0.306	246	0.9486	
R ²	0.9164	0.077	39.3	0.9152*	0.904
Entropy	0.8982	1.60	29.2	0.8980	0.954
CP	0.8693	0.739	21.7	0.8636	0.668

In the last column we give the best regression coefficients as reported in ref. [44] in which some 40 molecular descriptors were tested against some twenty physicochemical properties of octane isomers. We have employed two descriptors, *a* and *b*, hence the comparison may be somewhat biased. In order to make a more balanced comparison we included in the adjacent to the last column the regression coefficient when only the dissection parameter *a* is used. In the case of the quadratic mean radius we have used quadratic, rather than linear regression, (which yields low *r* value of 0.770). As we see from the short comparison only in the case of the entropy *S* better molecular descriptors than *a*, or *a* and *b* combined were reported in ref. [44].

The regression coefficient of around 0.900 is not necessarily satisfactory, though one should keep in mind that we are correlating properties for isomers which are molecules of the same size, thus making regression more difficult to fit, because the dominant size contribution has been effectively eliminated from considerations. Nevertheless, as we see from the above comparison the dissection parameters *a* alone,

and a , b jointly, produced much better regression for the quadratic mean radius R^2 and the critical pressure (CP) than hitherto available alternative descriptors.

The correlation power of new descriptors (a , b) has well been illustrated for the octane steric factors that have hitherto eluded simple correlation, or correlation based on few descriptors only. This definitely demonstrates use of (a , b) descriptors, which is further emphasized by the fact that the dissection parameters (a , b) are integers, the most simplest type of molecular descriptors, according to the classification of Balaban.⁴⁵ If we compare (a , b) with other integer molecular descriptors, the Wiener number,⁴⁶ the Hosoya's Z topological index,⁴⁷ and the hyper-Wiener index,^{48,49} we see that dissection parameters (a , b) are larger integers. This allows them to fit data with a greater precision that typifies the real valued topological indices, like the connectivity index ${}^1\chi$,²⁵ Balaban's J index,⁵⁰ and similar indices.

Here we will illustrate correlation with Pitzer constants (P) for octanes. Linear correlation based on a as the only descriptor already gives satisfactory results for octane:

$$P = -0.00005086 a + 0.411422 \quad (1)$$

with $r = 0.9787$, $s = 0.0064$, and $F = 342$. The correlation is shown in Fig. 3. The quadratic regression using the parameter a is marginally better than the linear regression. For the quadratic regression (shown in Fig. 4) we have:

$$P = -0.00008181 a + 0.00000001 a^2 + 0.43151 \quad (2)$$

with $r = 0.9858$, $s = 0.0054$ and $F = 243$.

The correlation of the parameter b against the parameter a for the 18 isomers of octane is shown in Fig. 5. The correlation between the two descriptors shows considerable duplication: $r = 0.9981$, $s = 34.71$, and $F = 4228$. It appears that one of the descriptors suffices for regression, while the other does not bring much novelty. One can combine the two descriptors as a combination ($a + 2b$) which represents a result obtained by further dissection of the edge as a fragment. However, the descriptor ($a + 2b$) does not improve the result over the already found regression using a as a single descriptor.

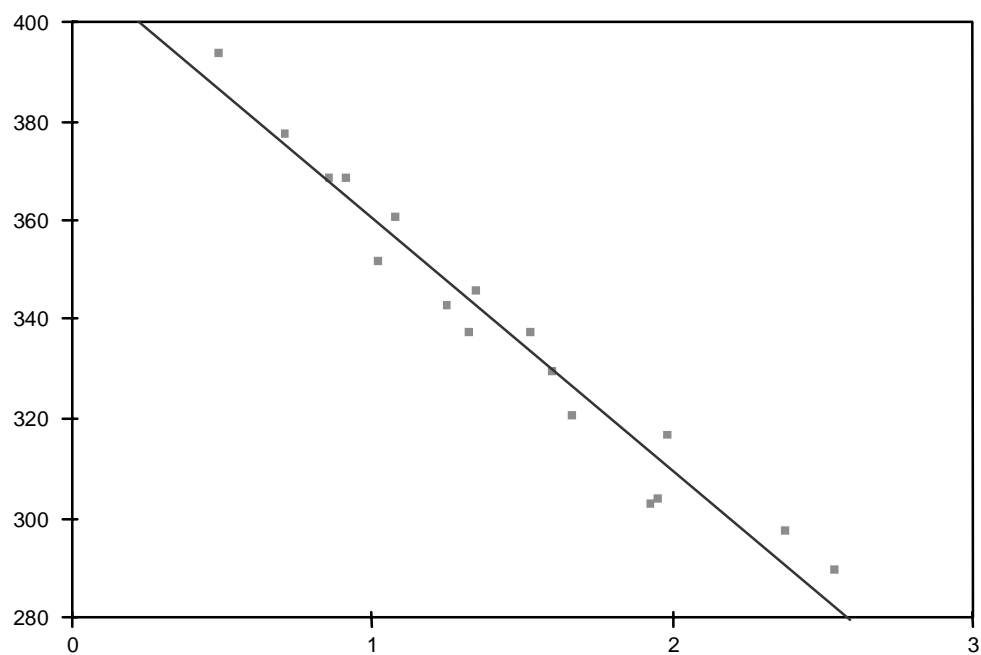


Fig. 3 Linear regression of Pitzer factor of octane against a

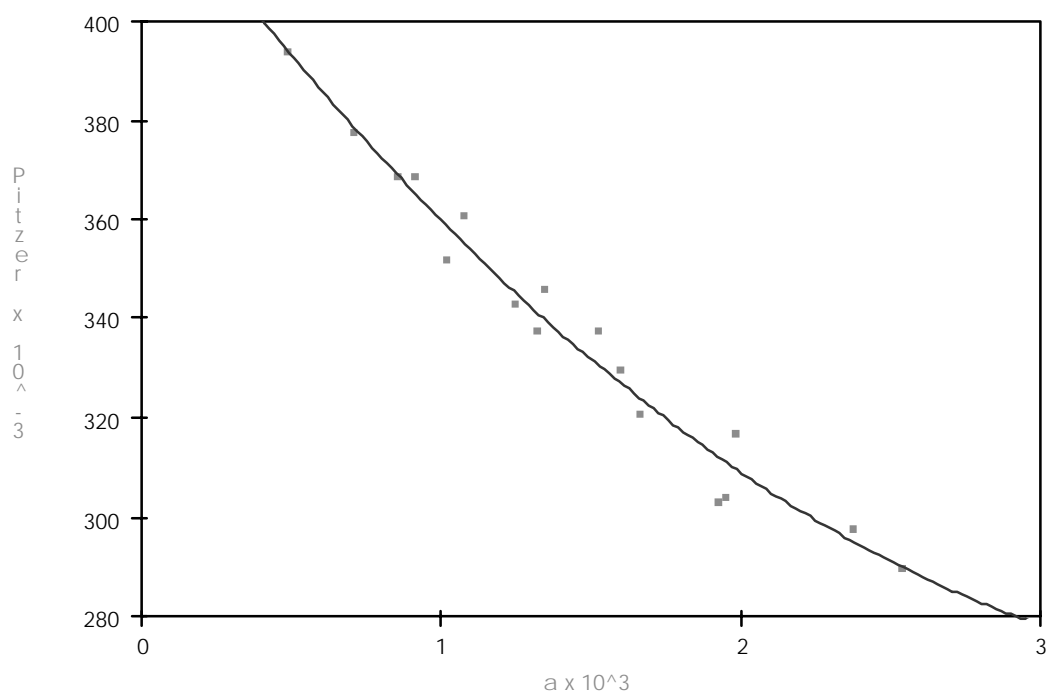


Fig. 4 Quadratic regression of Pitzer factor of octane against a

Use of the descriptor b alone gives results similar to those obtained with descriptor a :

$$P = -0.00010074 b + 0.00000001 b^2 + 0.440409 \quad (3)$$

with statistical parameters: $r = 0.9787$, $s = 0.0061$ and $F = 159$.

Even this result is better than regression using both a and b as descriptors, which gives:

$$P = -0.00005218 a + 0.00000183 b + 0.411096 \quad (4)$$

with $r = 0.9787$, $s = 0.0066$ and $F = 159$.

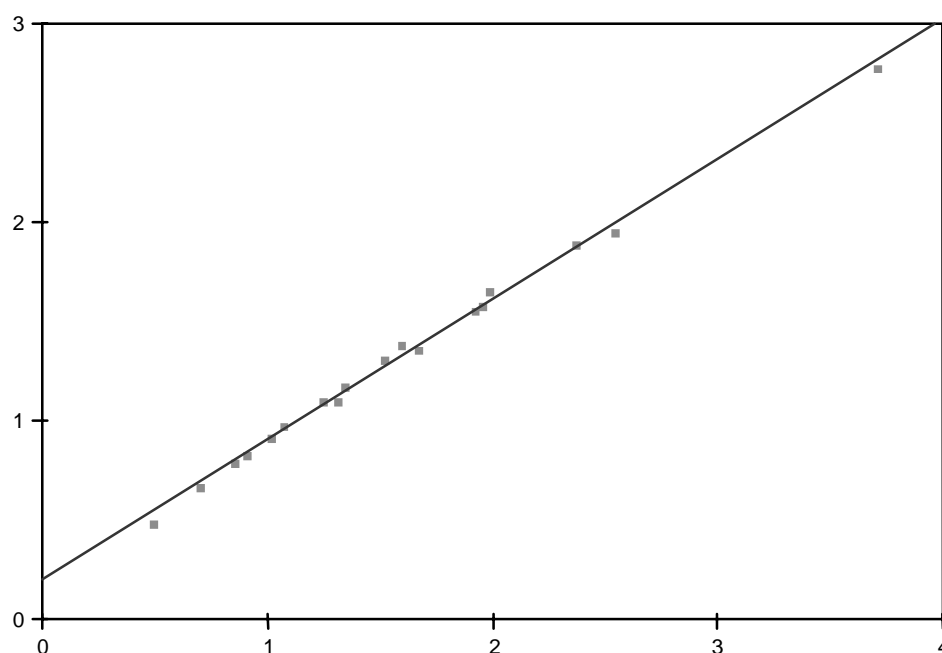


Fig. 5 The correlation of the parameter b against the parameter a for the 18 isomers of octane

Regression for Steric Factors

Recently introduced shape indices^{2,3} p_2/w_2 , p_3/w_3 , p_4/w_4 were successfully correlated with several molecular properties. Here we wish to consider in particular the regressions with the steric factors. The the statistical parameters when using two and three shape indices respectively are shown in Table 5. The results are comparable with

those based on the dissection parameters (a, b), but even three shape indices do not give regression as good as that based on the dissection parameters.

Table 5 Statistical parameters for path/walk descriptors

Descriptors	r	s	F
$p_2/w_2, p_3/w_3$	0.9693	0.453	109
$p_2/w_2, p_3/w_3, p_4/w_4$	0.9710	0.457	71

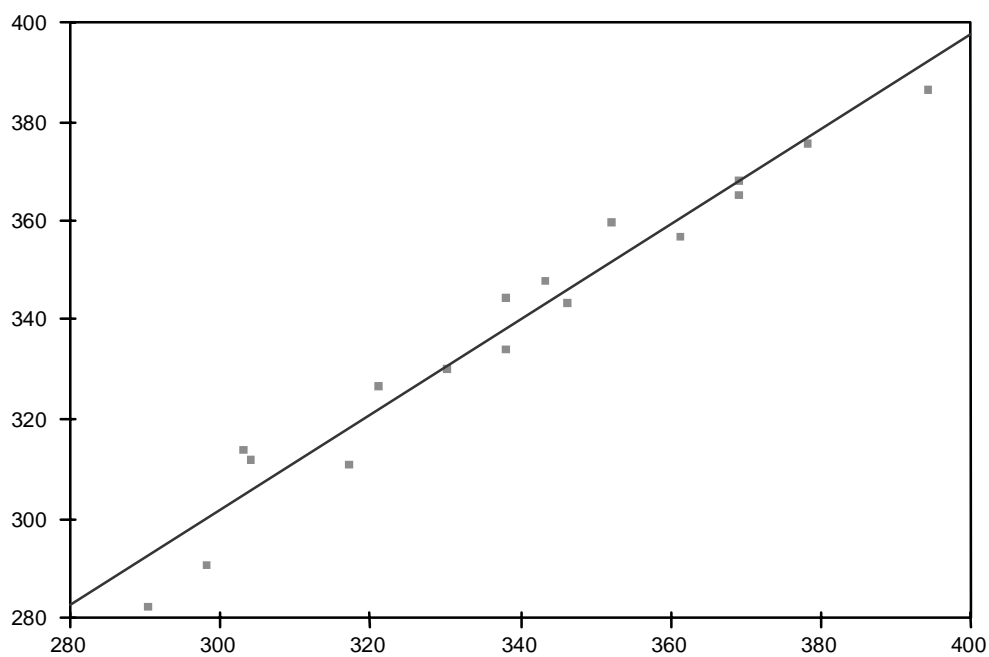


Fig. 6 The linear regression of the calculated values of the steric factor against the experimental values

A quadratic relation of the hyper-Wiener index WW with the steric factors is quite satisfactory: $r = 0.9821$, $s = 0.346$ and $F = 191$. This compares well with the quadratic

regression based on either the parameter a alone, or b alone ($r = 0.9715$ and $r = 0.9776$ respectively) and approaches the regression based on (a, b) . In Table 4 we report the experimental and the calculated values for steric factors of octanes as obtained in the regression using the parameters (a, b) . The regression is shown in Fig. 6.

Table 6 Experimental values for steric factors, the calculated values and the residuals of a regression using the dissection parameters (a, b) .

Molecule	Steric (exp)	Steric (calc)	Residual
n-octane	0	-0.297	0.297
2-methylheptane	0.608	0.489	0.119
3-methylheptane	1.216	1.076	0.140
4-methylheptane	1.216	1.264	-0.048
3-ethylhexane	1.824	1.984	-0.160
2,2-dimethylhexane	1.397	1.851	-0.454
2,3-dimethylhexane	2.818	2.623	0.195
2,4-dimethylhexane	1.824	2.376	-0.552
2,5-dimethylhexane	1.216	1.593	-0.376
3,3-dimethylhexane	2.794	2.782	0.012
3,4-dimethylhexane	3.513	3.259	0.254
2-methyl, 3-ethylpentane	3.513	3.581	-0.068
3-methyl, 3-ethylpentane	4.191	3.660	0.531
2,2,3-trimethylpentane	4.493	4.632	-0.139
2,2,4-trimethylpentane	3.743	3.466	0.277
2,3,3-trimethylpentane	*	*	*
2,3,4-trimethylpentane	4.598	4.504	0.094
2,2,3,3-tetramethylbutane	6.501	6.622	-0.121

The largest residuals are obtained for 3-methyl-3-ethylpentane, 2,4-dimethylhexane and 2,2-dimethylhexane. The experimental value of the steric factor for 2, 3, 3-trimethylpentane was not reported. The equation for the correlation of the calculated and the experimental values of the steric factor is very close to equation $y = x$ (linear coefficient is 0.97233 and the constant is 0.07399). The coefficient of the correlation is 0.9861, the standard error 0.292 and the Fisher ratio $F = 572$.

Correlation of (a, b) with other Topological Indices

The dissection parameters (a, b) do not correlate with most of other topological indices. This could be expected in view that steric factor could not be well correlated with the existing topological indices. We do find however that (a, b) correlate quite well with WW index, the hyper-Wiener index. The parallelism between (a, b) and WW is confirmed by correlating WW with a, b, which gives the linear regression equation:

$$WW = 0.5305 a - 0.879 b + 576.54 \quad (5)$$

and the statistical parameters: $r = 0.9494$, $s = 26.5$, and $F = 69$. If so computed WW is plotted against WW we have a quadratic regression equation:

$$WW_{\text{calc}} = 1.9030 WW - 0.0018 WW^2 - 121.11 \quad (6)$$

and the statistical parameters : $r = 0.9686$, $s = 19.9$, and $F = 114$.

Hence, we may expect that the dissection parameters (a, b) will be of interest in correlations in which hyper-Wiener index WW has been found suitable. The WW index was tested against doze physicochemical properties of octanes,⁴¹ however, as a single descriptor it was not better than the Wiener number W, the JJ, or the leading eigenvalue of the Wiener matrix. Only in combination with other indices WW resulted in some fine regression. It seems therefore that the novel descriptors, the dissection parameters (a, b), could be of interest in regression in which they are similarly combined with other descriptors, in particular with the descriptors that combined with WW produced very good correlations, as shown in ref. [49]. We hope to explore these novel possibilities but such work is outside the scope of the present report.

Open Problems

In conclusion we may say that one is justified to extend the present study and explore properties of novel molecular descriptors. We already have preliminary results for larger trees and smaller cyclic graphs. In addition we obtained the recursion relations for selected homologous series of molecules. The particularly simple expression holds for n-alkanes and 2-ethylalkanes. For the former, $a_n = b_n = 6n$, while for the latter we have separate recursion for a_n and b_n :

$$a_{n+1} = 3 a_n$$

$$b_{n+1} = 3 b_n + 10 n$$

For trees we have $a_n > b_n$, except for chains when $a_n = b_n$. In cyclic compounds, with or without the pending branches, we can have $a_n > b_n$, $a_n < b_n$, and $a_n = b_n$. This last relation always holds for monocyclic C_n structures.

Among the open problems the very important is the question of the uniqueness of (a, b) characterization of trees. If this can be proved there would be no need for exhaustive search for the smallest pair of trees with duplicate values for (a, b). While (a, b) characterization may be unique for trees, the situation may not hold for cyclic graphs.

Table 7 The contribution to the dissection parameters (a, b) of the symmetry nonequivalent carbon atoms of different hexane isomers

Isomer	atom 1	atom 2	atom 3	atom 4	atom5
n-octane	18a + 18b	7a + 6b	2a + 3b		
2-methyl	18a + 18b	4a + 2b	2a + 3b	10a + 6b	26a + 21b
3-methyl	26a + 21b	7a + 6b	a + 2b	18a + 18b	
2,3-dimethyl	26a + 21b	4a + 2b			
2,2-dimethyl	26a + 21b	3a + b	10a + 6b	40a + 24b	

Another question that merits attention is the problem of local variations of (a, b). Because the parameters are additive in terms of Ulam's subgraphs one can partition the

molecular (a, b) to individual atoms. In Table 7 we illustrate such partitioning for the individual (symmetry non-equivalent) atoms of five hexane isomers. As we see from these few illustrations the contributions of the terminal atoms is much greater than that of the internal atoms. There is here some parallelism with the connectivity index χ , which assigns to terminal CC bonds greater weight than to the internal CC bonds. We can contrast this to the components entering the construction of the Wiener index W , and the hyper-Wiener index, where the internal bonds make a greater contribution.

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Povzetek

Disekcija grafov, ki je vpeljana pred dvajsetimi leti, daje karakterizacijo molekularnih grafov s celimi števili. Ta pristop, ki vnaša nekatera matematična vprašanja, omogoča uvajanje novih strukturnih deskriptorjev, ki so potencialno zanimivi za QSAR študije. V tem delu je disekcija grafov ponovno raziskana in nekaj napak zgodnejših objav je popravljenih. Novi deskriptorji, dobljeni s procesom disekcije, so ilustrirani na izbranih lastnostih oktanov.