

Restricted random walks on graphs

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Summary. In the first part of this contribution we outline the construction of a novel matrix associated with a graph, the entries of which give the probability of a random walk over the graph G starting at site i to reach site j in D_{ij} steps. Here D_{ij} is the distance between vertices i, j . The derived matrices, to be referred to as restricted random walk matrices and labeled as RRW matrices, are non-symmetric, for trees the entries being of the form $1/p$, where p is an integer equal to 1 or larger. In the second part of the report we consider a few invariants of the RRW matrices. We will illustrate the use of one such invariant in a regression analysis. We consider the variations of the entropies in isomeric octanes with skeletal changes. The derived regression, based on a single descriptor, yields the standard error of $1.26 \text{ cal K}^{-1} \text{ mol}^{-1}$ that is the smallest yet reported in the literature.

Key words: Graphs – Restricted random walks

1 Introduction

Recently we initiated a systematic search for the matrices that can be associated with molecular graphs and serve as a source for the construction of novel graph invariants that may be of use in structure–property analysis. This effort resulted in several novel matrices of potential interest in structure–property–activity studies. The Wiener matrix [1] is based on a particular generalization of a partitioning of the Wiener number [2], a widely used molecular topological descriptor. The Hosoya matrix [3] was similarly derived by partitioning Hosoya's Z number [4], another important topological index. In yet another study, which applies to graphs embedded on regular grids (in two or three dimensions, such as the graphite network or diamond grid, respectively) the notions of the geometrical and the topological distance were combined in producing novel

This paper is dedicated to Professor D.J. Klein (Texas A&M at Galveston), a pioneer of the overlapping areas of group theory, graph theory and quantum theory.

matrices that show some promise in the characterization of different molecular conformations [5].

In this paper we will outline the construction of yet another novel matrix associated with graphs, the elements of which are determined by considering random walks. A selected invariant of such matrices shows considerable promise in structure–property studies.

2 Motivation

The interest in novel matrices associated with graphs originates with a hope that some such matrix can generate structural invariants that can improve on the existing simple and multiple regressions for different structural properties. Recently we have reported some 750 regressions derived for the 18 isomers applied to some 20 physicochemical properties and tested some 40 molecular (mathematical) descriptors in simple regressions (based on a single independent variable) [6]. The results of this rather ambitious survey of simple structure–property regressions revealed several interesting points. First, from the pool of some 40 descriptors at most half a dozen (and few combinations of these descriptors) emerged again and again as the best molecular descriptors. These best descriptors include the connectivity index χ [7], the Hosoya Z topological index [4] and the Wiener number W [2]. Another interesting result of the survey is the finding that for some molecular properties many descriptors can produce a fair regression, while for other properties none of the 40 descriptors (as a single variable) gives a satisfactory regression. The Pitzer acentric factor [8] is an example of the former, and the critical temperatures and the critical pressures are an illustration of the latter. We should emphasize that the above analysis was confined to molecules of the same size (i.e., having the same number of carbon atoms and CC bonds). Variations of the properties within such a group demand that the descriptors are sensitive to variations in the skeletal branching. It is generally not difficult to design descriptors that will adequately describe the dominant role of the molecular size on the properties. Variations of the properties with the molecular shape are much more difficult to account for [9].

Hence, there is a continuing interest in the search for novel molecular descriptors. One hopes that such a search may result in the design of descriptors that show a significant improvement over the performance of the earlier descriptors. Although regression analysis does not produce a causal relationship, the use of theoretical descriptors may signal structural components that are relevant for a particular molecular property and this may contribute to better molecular models. However, the challenges ahead for those interested in the design of novel structural descriptors are considerable. It is not sufficient just to announce a novel descriptor, the designer should also demonstrate that a novel descriptor can yield a better, simple or multiple, regression than given by the existing descriptors, while the descriptor still has a relatively simple structural interpretation. That indeed this is not to be an easy task has been confirmed by recent work of Kartizky and Gordeeva [10] who screened a large number of topological indices in analyzing several structure–activity relationships and have again found the same “classic” descriptors (the connectivity index, the Hosoya Z index and the Wiener W number) as the dominant molecular descriptors.

3 Restricted random walks

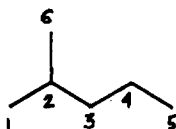
A random walk (or sometimes also referred to as a drunkard's walk) along a one-dimensional path that is divided into n segments starts at one point and using chance process continues (left or right), segment by segment, until it reaches either of the limiting ends of the path [11]. It can be easily generalized to two dimensional networks, and even higher-dimensional grids, with several end points. The problem to solve in such cases is that of finding the probability, starting at any of the segments (or crossroads in the case of two dimensions), that a walker will reach one of the ends (home or a bar in the case of a drunkard!). There are no restrictions on the number of steps required to reach either of the end sites.

We will, however, consider random walks over graphs but will restrict the number of steps that are allowed. The restriction we impose on the number of steps is determined by the distance of the vertices considered, as will be illustrated below. Besides the probabilities for restricted random walks between vertices i and j , a related idea is to consider unrestricted random walks, which can be defined as

$$P_{i \rightarrow j} = \begin{cases} \text{the probability that a random walk leaving site } i \\ \text{will reach site } j \text{ before returning to } i. \end{cases}$$

As noted in [11, 54] this is just the inverse of the resistance (or resistance distance [12]) between i and j . The matrix of $P_{i \rightarrow j} = 1/\Omega_{ij}$ has already been noted as a possibly interesting characteristic for molecular graphs [13].

Let us outline our approach for the graph of 2-methylpentane:



As we have said, the number of steps in a random walk is restricted by the distance of the vertices considered. For example, if we start at vertex 1 and want to arrive at vertex 4, which is three bonds away, we allow only random walks of length three. For smaller molecules, such as 2-methylpentane, we can list all such walks and find the required probability by brute force. Thus, by starting at vertex 1 the following are all the possible walks having length three:

$$1-2-3-4; \quad 1-2-3-2; \quad 1-2-6-2; \quad 1-2-1-2.$$

Hence, in all, there are four such walks, but only one (1-2-3-4) indicates a success: thus the probability for reaching vertex 4 starting from 1 in three steps is $1/4$. If we consider the reverse of this, the probability of reaching vertex 1 starting from vertex 4 (in three steps), we have the following possible walks:

$$4-3-2-1; \quad 4-3-2-6; \quad 4-3-2-3; \quad 4-3-4-3; \quad 4-3-4-5; \quad 4-5-4-3; \quad 4-5-4-5.$$

Now in all there are seven walks, one of which represents a success; hence the probability is $1/7$.

By this process we were able to assign to a pair of vertices (i, j) a number; hence we can now build a matrix with the entries in such a matrix given by the calculated probabilities. Thus in the case of 2-methylheptane for the element (1, 4) we have $1/4$ and for the element (4, 1) we have $1/7$. We will refer to such matrices as restricted random walk or RRW matrices and will in the next section illustrate a few such for

the selected isomers of octane in order to show the form of RRW matrices. Observe that the derived matrices are not symmetric.

4 Illustrations

In Table 1 we show RRW matrices for n alkanes and in Table 2 we show RRW matrices for four (out of 18) isomers of octane. In general, the largest entries in each row or column are those close to the main diagonal. The RRW matrices for n -alkanes are centrosymmetric, i.e., an element (i, j) is equal to element $(n + 1 - i, n + 1 - j)$, which would have the same labels if we would reverse the labeling of the rows and the columns, i.e., if we would count rows from the right and

Table 1. The restricted random walks matrices for n -alkanes

$\begin{matrix} n\text{-propane} \\ \left(\begin{array}{ccc} 0 & 1 & 1/2 \\ 1/2 & 0 & 1/2 \\ 1/2 & 1 & 0 \end{array} \right) \end{matrix}$	$\begin{matrix} n\text{-butane} \\ \left(\begin{array}{cccc} 0 & 1 & 1/2 & 1/3 \\ 1/2 & 0 & 1/2 & 1/3 \\ 1/3 & 1/2 & 0 & 1/2 \\ 1/3 & 1/2 & 1 & 0 \end{array} \right) \end{matrix}$
$\begin{matrix} n\text{-pentane} \\ \left(\begin{array}{ccccc} 0 & 1 & 1/2 & 1/3 & 1/6 \\ 1/2 & 0 & 1/2 & 1/3 & 1/6 \\ 1/4 & 1/2 & 0 & 1/2 & 1/4 \\ 1/6 & 1/3 & 1/2 & 0 & 1/2 \\ 1/6 & 1/3 & 1/2 & 1 & 0 \end{array} \right) \end{matrix}$	$\begin{matrix} n\text{-hexane} \\ \left(\begin{array}{cccccc} 0 & 1 & 1/2 & 1/3 & 1/6 & 1/10 \\ 1/2 & 0 & 1/2 & 1/3 & 1/6 & 1/10 \\ 1/4 & 1/2 & 0 & 1/2 & 1/4 & 1/7 \\ 1/7 & 1/4 & 1/2 & 0 & 1/2 & 1/4 \\ 1/10 & 1/6 & 1/3 & 1/2 & 0 & 1/2 \\ 1/10 & 1/6 & 1/3 & 1/2 & 1 & 0 \end{array} \right) \end{matrix}$
$\begin{matrix} n\text{-heptane} \\ \left(\begin{array}{cccccc} 0 & 1 & 1/2 & 1/3 & 1/6 & 1/10 & 1/20 \\ 1/2 & 0 & 1/2 & 1/3 & 1/6 & 1/10 & 1/20 \\ 1/4 & 1/2 & 0 & 1/2 & 1/4 & 1/7 & 1/14 \\ 1/8 & 1/4 & 1/2 & 0 & 1/2 & 1/4 & 1/8 \\ 1/14 & 1/7 & 1/4 & 1/2 & 0 & 1/2 & 1/4 \\ 1/20 & 1/10 & 1/6 & 1/4 & 1/2 & 0 & 1/2 \\ 1/20 & 1/10 & 1/6 & 1/4 & 1/2 & 1 & 0 \end{array} \right) \end{matrix}$	
$\begin{matrix} \text{octane} \\ \left(\begin{array}{cccccc} 0 & 1 & 1/2 & 1/3 & 1/6 & 1/10 & 1/20 & 1/35 \\ 1/2 & 0 & 1/2 & 1/3 & 1/6 & 1/10 & 1/20 & 1/35 \\ 1/4 & 1/2 & 0 & 1/2 & 1/4 & 1/7 & 1/14 & 1/25 \\ 1/8 & 1/4 & 1/2 & 0 & 1/2 & 1/4 & 1/8 & 1/15 \\ 1/15 & 1/8 & 1/4 & 1/2 & 0 & 1/2 & 1/4 & 1/8 \\ 1/25 & 1/14 & 1/7 & 1/4 & 1/2 & 0 & 1/2 & 1/4 \\ 1/35 & 1/20 & 1/10 & 1/6 & 1/3 & 1/2 & 0 & 1/2 \\ 1/35 & 1/20 & 1/10 & 1/6 & 1/3 & 1/2 & 1 & 0 \end{array} \right) \end{matrix}$	

columns from the bottom. There are some other regularities to be observed. In the case of n -alkanes, as we move along each of the diagonals parallel to the main diagonal of the matrix the entries decrease. After they reach the value $1/2^d$ they remain constant. Here d is the "distance" of the diagonals from the main diagonal.

Table 2. The restricted random walks matrices for several octane isomers

$$\begin{array}{c} \text{2-methylheptane} \\ \left(\begin{array}{cccccccc} 0 & 1 & 1/3 & 1/4 & 1/11 & 1/16 & 1/42 & 1/3 \\ 1/3 & 0 & 1/3 & 1/4 & 1/11 & 1/16 & 1/42 & 1/3 \\ 1/5 & 1/2 & 0 & 1/2 & 1/5 & 1/8 & 1/20 & 1/5 \\ 1/9 & 1/4 & 1/2 & 0 & 1/2 & 1/4 & 1/9 & 1/9 \\ 1/15 & 1/7 & 1/4 & 1/2 & 0 & 1/2 & 1/4 & 1/15 \\ 1/21 & 1/10 & 1/6 & 1/3 & 1/2 & 0 & 1/2 & 1/21 \\ 1/21 & 1/10 & 1/6 & 1/3 & 1/2 & 1 & 0 & 1/21 \\ 1/3 & 1 & 1/3 & 1/4 & 1/11 & 1/16 & 1/42 & 0 \end{array} \right) \end{array}$$

$$\begin{array}{c} \text{2,3-dimethylhexane} \\ \left(\begin{array}{cccccccc} 0 & 1 & 1/3 & 1/5 & 1/12 & 1/23 & 1/3 & 1/5 \\ 1/3 & 0 & 1/3 & 1/5 & 1/12 & 1/23 & 1/3 & 1/5 \\ 1/6 & 1/3 & 0 & 1/3 & 1/6 & 1/13 & 1/6 & 1/3 \\ 1/9 & 1/6 & 1/2 & 0 & 1/2 & 1/6 & 1/9 & 1/6 \\ 1/12 & 1/7 & 1/3 & 1/2 & 0 & 1/2 & 1/12 & 1/7 \\ 1/12 & 1/7 & 1/3 & 1/4 & 1 & 0 & 1/12 & 1/7 \\ 1/3 & 1 & 1/3 & 1/5 & 1/12 & 1/23 & 0 & 1/5 \\ 1/6 & 1/3 & 1 & 1/3 & 1/6 & 1/13 & 1/6 & 0 \end{array} \right) \end{array}$$

$$\begin{array}{c} \text{2-methyl-3-ethylpentane} \\ \left(\begin{array}{cccccccc} 0 & 1 & 1/3 & 1/5 & 1/13 & 1/3 & 1/5 & 1/13 \\ 2/3 & 0 & 1/3 & 1/5 & 1/13 & 1/3 & 1/5 & 1/13 \\ 1/7 & 1/3 & 0 & 1/3 & 1/7 & 1/7 & 1/3 & 1/7 \\ 1/9 & 1/4 & 1/2 & 0 & 1/2 & 1/9 & 1/4 & 1/9 \\ 1/9 & 1/4 & 1/2 & 1 & 0 & 1/9 & 1/4 & 1/9 \\ 1/3 & 1 & 1/3 & 1/5 & 1/13 & 0 & 1/5 & 1/13 \\ 1/9 & 1/4 & 1/2 & 1/4 & 1/9 & 1/9 & 0 & 1/2 \\ 1/9 & 1/4 & 1/2 & 1/4 & 1/9 & 1/9 & 1 & 0 \end{array} \right) \end{array}$$

$$\begin{array}{c} \text{2,3,3-trimethylpentane} \\ \left(\begin{array}{cccccccc} 0 & 1 & 1/3 & 1/6 & 1/13 & 1/3 & 1/6 & 1/6 \\ 1/3 & 0 & 1/3 & 1/6 & 1/13 & 1/3 & 1/6 & 1/6 \\ 1/7 & 1/4 & 0 & 1/4 & 1/7 & 1/7 & 1/4 & 1/4 \\ 1/9 & 1/5 & 1/2 & 0 & 1/2 & 1/9 & 1/5 & 1/5 \\ 1/9 & 1/5 & 1/2 & 1 & 0 & 1/9 & 1/5 & 1/5 \\ 1/3 & 1 & 1/3 & 1/6 & 1/13 & 0 & 1/6 & 1/6 \\ 1/7 & 1/4 & 1 & 1/4 & 1/7 & 1/7 & 0 & 1/4 \\ 1/7 & 1/4 & 1 & 1/4 & 1/7 & 1/7 & 1/4 & 0 \end{array} \right) \end{array}$$

Brute force calculation of the matrix elements for RRW is error prone. To obtain the elements of the RRW matrix we find it best to construct the adjacency matrix first and then calculate A^n powers of the adjacency matrix that contain information on the number of walks of length n for every vertex [14]. From the higher powers of A one can extract the number of walks of any length, and hence construct the RRW matrix. For example, to obtain the elements (1, 4) and (4, 1) for RRW of 2-methylpentane we raise the adjacency matrix of 2-methylpentane to the third power and construct the row sums for row 1 and row 4, respectively:

A	A^3	Row Sum
$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 3 & 0 & 1 & 0 & 0 \\ 2 & 0 & 4 & 0 & 2 & 1 \\ 0 & 4 & 0 & 3 & 0 & 0 \\ 1 & 1 & 3 & 0 & 2 & 0 \\ 0 & 1 & 0 & 2 & 0 & 0 \\ 0 & 3 & 0 & 1 & 0 & 0 \end{pmatrix}$	4 9 7 7 3 4

We see that the row sums, which give the count of all walks starting at the vertex for the selected row, for vertex 1 and vertex 4 give values 4 and 7, respectively. From the matrix A^3 we can obtain the elements for RRW for all pairs of vertices separated by three bonds. Thus, in addition to (1, 4) and (4, 1) we can also extract the following entries of RRW of 2-methylheptane:

$$(2, 5) = 1/9, \quad (5, 2) = 1/3 \quad \text{and} \quad (4, 6) = 1/7, \quad (6, 4) = 1/4.$$

The algorithm for construction of the RRW matrices thus is based on information from the adjacency matrix and the distance matrix. The powers of the adjacency matrix give walks of increasing length, while the elements of the distance matrix indicate the restrictions on the length of the walks. A computer program that implements such an algorithm is under preparation [15].

5 RRW matrix invariants

Once a matrix is assigned to a graph one can extract various invariants from such a matrix to be tested as potential molecular descriptors. Besides the standard matrix invariants such as the eigenvalues (spectrum), the determinant, and the coefficients of the characteristic polynomial, these also include path additive quantities. These are constructed in the following way; identify for the molecular graph considered all paths of length 1 (i.e. bonds) and add all such contributions. Next, consider all paths of length 2 (two consecutive bonds) and add all entries in the matrix corresponding to such. Continue the process for ever-increasing path lengths until all entries are exhausted. For n -alkanes construction of such path additive quantities is particularly simple because (with the natural numbering) vertices at the same distance are located along the diagonals parallel to the main diagonal. All adjacent vertices have entries next to the main diagonal, contributions to paths of length two are located on the second diagonal parallel to the main

diagonal, and so on. Thus in the case of n -octane we have:

Paths of length 1: $R_1 = 2(1 + 1/2 + 1/2 + 1/2 + 1/2 + 1/2 + 1/2) = 8.00000$

paths of length 2: $R_2 = 2(1/2 + 1/3 + 1/4 + 1/4 + 1/4 + 1/4) = 3.66667$

paths of length 3: $R_3 = 2(1/3 + 1/6 + 1/7 + 1/8 + 1/8) = 1.78571$

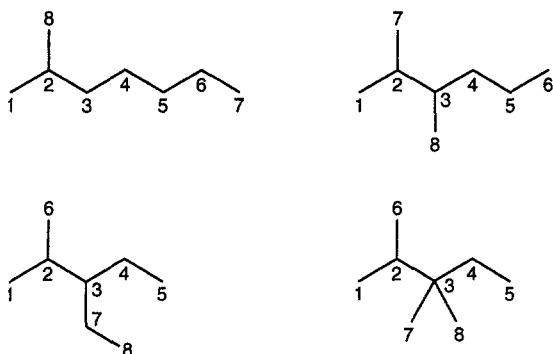


Fig. 1. Labeling of vertices in selected isomers of octane

Table 3. The path additive sequences for the 18 isomers of octane. The last entry for each molecule gives the sum of all the path numbers and correspond to the path identification number

	<i>n</i> -octane	2M	3M	4M	3E	22MM
R_0	8.00000	8.00000	8.00000	8.00000	8.00000	8.00000
R_1	3.66667	4.01667	4.00000	3.93333	4.03333	4.45000
R_2	1.78571	1.69210	2.09841	2.04194	2.41819	1.60000
R_3	0.80952	0.69432	0.75146	1.00709	1.07003	0.62500
R_4	0.38000	0.34405	0.37527	0.25589	0.28431	0.37500
R_5	0.18000	0.14285	0.08333	0.07407		
R_6	0.02857					
ID _R	14.85047	14.97999	15.30847	15.31232	15.80586	15.05000
	23MM	24MM	25MM	33MM	34MM	2M3E
R_0	8.00000	8.00000	8.00000	8.00000	8.00000	8.00000
R_1	4.23333	4.31667	4.43667	4.33333	4.33333	4.430476
R_2	2.30153	1.97448	1.62626	2.26374	2.65385	2.62051
R_3	0.73945	0.80651	0.59893	0.73026	0.77149	0.97436
R_4	0.25362	0.23529	0.47059	0.08333	0.11765	
ID _R	15.52793	15.33295	15.06245	15.51066	15.87632	15.89963
	3M3E	223MMM	224MMM	233MMM	234MMM	2233MMMM
R_0	8.00000	8.00000	8.00000	8.00000	8.00000	8.00000
R_1	4.47857	4.82143	4.74762	4.86190	4.70476	5.35714
R_2	2.389524	2.45739	1.43603	2.75629	2.47912	2.57143
R_3	0.66667	0.49123	0.77733	0.37607	0.61538	
ID _R	16.04048	15.77005	14.96098	15.99426	15.79926	15.92857

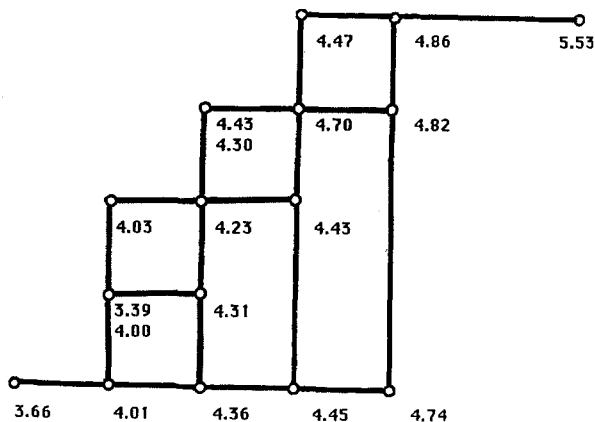


Fig. 2. The plot of R_1 on the p_2, p_3 coordinate grid

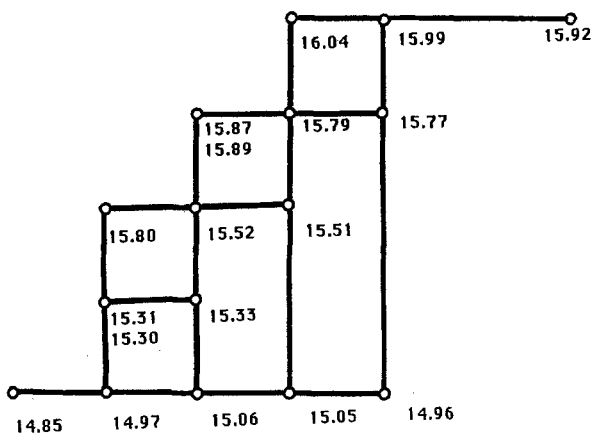


Fig. 3. The plot of the identification number ID_R on the p_2, p_3 coordinate grid

and so on. Figure 1 shows the labeling of vertices in selected isomers of octane. In Table 3 we give the corresponding path sequences for the 18 isomers of octanes. The last entry for each molecule is the sum of all lengths. The numbers correspond to the molecular ID (identification) number [16], although these were introduced for different matrices initially. The first entry in the path sequences gives the number of vertices (and is constant for isomers). The second entry represents a bond additive quantity and is reminiscent of the connectivity index (which is also bond additive). Both, the bond additive R_1 and the ID_R number show a regular variation for the isomers if plotted on the p_2, p_3 coordinate grid, a suggested template to detect the regularities in isomeric variations [17], as illustrated in Figs. 2 and 3.

6 Isomeric variation of entropy

In Table 4 we show the experimental entropies for the isomers of octanes (the second column). In Fig. 4 we plot the experimental entropy against the bond additive invariant R_1 , whence a rather satisfactory regression results:

$$\text{entropy (cal K}^{-1} \text{ mol}^{-1}) = -11.028 R_1 + 153.679$$

Table 4. The experimental entropies of the octane isomers, the calculated entropies and the differences. The experimental values were taken from refero calorimetric values of entropies in $\text{cal K}^{-1} \text{mol}^{-1}$

Isomer	Entropy (exp.)	Entropy (calc.)	Difference
<i>n</i> -octane	111.67	113.243	- 1.57
2M	109.84	109.384	+ 0.46
3M	111.26	109.567	+ 1.69
4M	109.32	110.303	- 0.98
3E	109.43	109.200	+ 0.23
22MM	109.42	104.605	- 1.18
23MM	108.02	106.994	+ 1.03
24MM	106.98	106.075	+ 0.90
25MM	105.72	105.524	+ 0.20
33MM	104.74	104.789	- 0.05
34MM	106.51	105.89	+ 0.62
2M3E	106.06	106.207	- 0.15
3M3E	101.48	104.290	- 2.81
223MMM	101.31	100.509	+ 0.80
224MMM	101.09	101.323	- 0.23
233MMM	102.06	100.062	+ 2.00
234MMM	102.39	101.795	+ 0.59
2233MMMM	93.06	94.601	- 1.54

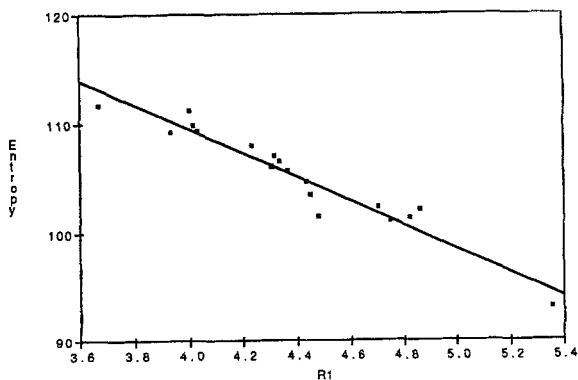


Fig. 4. The plot of the experimental entropies against R_1

with correlation coefficient $r = 0.964$ and the standard error $s = 1.265$. The computed entropies and the difference between the experimental and the calculated entropies are included in Table 4 (the third and fourth columns). How does this result compare with descriptions based on other topological indices? In Table 5 we collected the best dozen results for regression of the entropy for octane isomers using some 40 different topological descriptors [6]. As we see, the present result is not only the best but it is significantly better than all other hitherto tested molecular descriptors! This suggests that path invariants based on the RRW matrices may represent an important addition to the already available library of topological indices used in multiple regression analysis of the structure-property relationship.

Table 5. The regression coefficient r and the standard error s for the dozen best single variable regressions for the entropies of octane isomers (for details on the definition of the indices used see [6])

Descriptor	R	S
R_1	0.964	1.26
$\chi[1/2]$	0.954	1.40
$\chi[1]$	0.942	1.57
ID χ	0.938	1.61
ID $_A$	0.936	1.64
TI	0.931	1.71
ID	0.926	1.76
Y	0.919	1.84
I_{ED}	0.915	1.88
X	0.913	1.90
V	0.912	1.91
1χ	0.906	1.97
ID $_D$	0.906	1.98
$1/1\chi$	0.905	1.99
ID $_W$	0.901	2.02
EC	0.901	2.02

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