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Matrices of Reciprocal Distance, Polynomials and Derived Numbers

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Abstract: *Reciprocal distance matrix,* $\mathbf{RD}_e$, *and two new matrices based on reciprocal distance:* $\mathbf{RD}_p$, and $\mathbf{RD}_{Tr}$, *are considered with respect to their polynomials, eigenvalues and Wiener-type numbers. These descriptors are exemplified on selected sets of graphs. Correlational and separating aspects are also shown.*

Introduction

The matrix representation of a graph, **G**, was made, till the end of '80 years, by the adjacency, **A**, and distance, **D**, matrices.[1] For reasons which will be shown bellow, within this work, the distance matrix will be marked by $\mathbf{D}_e$ .On these two matrices, a list of topological indices (i.e. single number descriptors) has been devised. While the adjacency matrix accounts for "vicinal" interactions within a molecule, the distance matrix describes also interactions between the more remote atoms.

It is well known, however, that these interactions diminish with increasing the distance between atoms. This argument originated the *reciprocal distance matrix,*[2,3] $\mathbf{RD}_e$, whose

+ Author to whom correspondence should be addressed entries are defined as

$$[\mathbf{RD_e}]_{ij} = 1 / [\mathbf{D_e}]_{ij} \tag{1}$$

The half sum of its entries offers a Wiener number[4] analogue, called the Harary number,[2,3] in the honor of Frank Harary

$$H_{De} = (1/2) \sum_i \sum_j [\mathbf{RD_e}]_{ij} \tag{2}$$

One of us[5] has recently proposed new "reciprocal property" matrices: **RW** (on Wiener matrix[6,7]), **RSZ** (on Szeged matrix[8,9]), **RCJ** (on Cluj matrix[10,11]) and $\mathbf{RW}_{(A,D,1)}$ (reciprocal walk matrix - see also ref. 12). The Harary-type indices showed interesting correlating and separating ability.[5,13]

New matrices based on reciprocal distance

By analogy to $\mathbf{RD_e}$, another matrix, called $\mathbf{RD_p}$, was proposed[14]

$$[\mathbf{RD_p}]_{ij} = 1 / [\mathbf{D_p}]_{ij} \tag{3}$$

Matrices $\mathbf{D_e}$ and $\mathbf{D_p}$ have the same essential meaning: their entries collect all paths, of length **e / p,** included in the shortest path **(i,j)**. Matrix $\mathbf{D_p}$ is defined[14] as

$$[\mathbf{D_P}]_{ij} = \binom{[\mathbf{D_e}]_{ij} + 1}{2} \tag{4}$$

Matrices $\mathbf{D_e}$ and $\mathbf{D_p}$ are involved in the definition and calculation of Wiener,[4] W, and hyper-Wiener,[15] WW, indices,[14,16] I

$$I = (1/2) \sum_i \sum_j [\mathbb{D}_{e/p}]_{ij} \quad (5)$$

If the matrix is defined on edge (i.e. $\mathbb{D}_e$), $I = W$ and if it is defined on path (i.e. $\mathbb{D}_p$), $I = WW$. Relation **(5)** holds for both acyclic and cyclic structures.

Another general definition of hyper-Wiener number was given by Klein, Lukovits and Gutman,[17] which can be written[18] as

$$WW = (\mathrm{Tr}(\mathbb{D}_e^2) / 2 + W) / 2 \quad (6)$$

Relation **(6)** allows the calculation of WW in any graph, when W is evaluated from $\mathbb{D}_e$ (cf. eq **5**). Moreover, it could offer a **(3D)***WW* index,[11] by using the geometric distances for building a **(3D)**$\mathbb{D}$ matrix. Note that, the Wiener matrix,[6,7] $\mathbb{W}_{e/p}$, also giving the WW index, does not obey relation **(6)**.

Keeping in mind the meaning of relations **(1)**, **(3)** and **(6)**, we propose here two new matrices

$$[\mathbb{D}_{Tr}]_{ij} = \frac{2([\mathbb{D}_e]_{ij})^2}{1 + [\mathbb{D}_e]_{ij}} \quad (7)$$

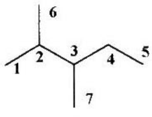
$$[\mathbb{RD}_{Tr}]_{ij} = 1 / [\mathbb{D}_{Tr}]_{ij} \quad (8)$$

Figure 1 illustrates the three distance-based matrices and their reciprocals, for the graph 2,3 - dimethylpentane, **1**.

A hyper-Harary number analogue

A hyper-Harary number can be constructed[5] as the half sum of entries in a square matrix, which collects a reciprocal property and is defined on path. (A "path definition" of an index is viewed as an extension of its "edge definition" - see refs. 14,15,19). Thus, it can be defined as

Figure 1. Distance-, and reciprocal distance-type matrices and derived Wiener-type indices for the graph 1



1

$\mathbb{D}_e$

	1	2	3	4	5	6	7
1	0	1	2	3	4	2	3
2	1	0	1	2	3	1	2
3	2	1	0	1	2	2	1
4	3	2	1	0	1	3	2
5	4	3	2	1	0	4	3
6	2	1	2	3	4	0	3
7	3	2	1	2	3	3	0

$W = D_e = (1/2)\sum_i \sum_j [\mathbb{D}_e]_{ij} = 46$

$\mathbb{RD}_e$

	1	2	3	4	5	6	7
1	0	1	1/2	1/3	1/4	1/2	1/3
2	1	0	1	1/2	1/3	1	1/2
3	1/2	1	0	1	1/2	1/2	1
4	1/3	1/2	1	0	1	1/3	1/2
5	1/4	1/3	1/2	1	0	1/4	1/3
6	1/2	1	1/2	1/3	1/4	0	1/3
7	1/3	1/2	1	1/2	1/3	1/3	0

$H = RD_e = (1/2)\sum_i \sum_j [\mathbb{RD}_e]_{ij} = 12$

$\mathbb{D}_p$

	1	2	3	4	5	6	7
1	0	1	3	6	10	3	6
2	1	0	1	3	6	1	3
3	3	1	0	1	3	3	1
4	6	3	1	0	1	6	3
5	10	6	3	1	0	10	6
6	3	1	3	6	10	0	6
7	6	3	1	3	6	6	0

$WW = D_p = (1/2)\sum_i \sum_j [\mathbb{D}_p]_{ij} = 83$

$\mathbb{RD}_p$

	1	2	3	4	5	6	7
1	0	1	1/3	1/6	1/10	1/3	1/6
2	1	0	1	1/3	1/6	1	1/3
3	1/3	1	0	1	1/3	1/3	1
4	1/6	1/3	1	0	1	1/6	1/3
5	1/10	1/6	1/3	1	0	1/10	1/6
6	1/3	1	1/3	1/6	1/10	0	1/6
7	1/6	1/3	1	1/3	1/6	1/6	0

$RD_p = (1/2)\sum_i \sum_j [\mathbb{RD}_p]_{ij} = 9.5333$

$\mathbb{D}_{Tr}$

	1	2	3	4	5	6	7
1	0	1	8/3	18/4	32/5	8/3	18/4
2	1	0	1	8/3	18/4	1	8/3
3	8/3	1	0	1	8/3	8/3	1
4	18/4	8/3	1	0	1	18/4	8/3
5	32/5	18/4	8/3	1	0	32/5	18/4
6	8/3	1	8/3	18/4	32/5	0	18/4
7	18/4	8/3	1	8/3	18/4	18/4	0

$D_{Tr} = (1/2)\sum_i \sum_j [\mathbb{D}_{Tr}]_{ij} = 64.4667$

$\mathbb{RD}_{Tr}$

	1	2	3	4	5	6	7
1	0	1	2	3	4	2	3
2	6	0	3	6	9	6	6
3	8	4	0	5	10	8	6
4	6	4	2	0	6	6	4
5	4	3	2	1	0	4	3
6	2	1	2	3	4	0	3
7	3	2	1	2	3	3	0

$RD_{Tr} = (1/2)\sum_i \sum_j [\mathbb{RD}_{Tr}]_{ij} = 10.2708$

$$H_{Mp} = (1/2)\sum_i\sum_j [\mathbf{RM}_p]_{ij} \qquad (9)$$

where $\mathbf{M}_p$ could be, e.g. $\mathbf{D}_p$. Relation **(9)** is equivalent to relation **(2)**.

Distance-based matrices obey relation **(6)**, as above mentioned. In this respect, a question could be put out: is it (or at least a formal identical relation) also obeied by the reciprocal distance matrix, $\mathbf{RD}_e$? If yes, what kind of number would offer? And further, could it be calculated by a relation of the type **(9)**, and how would look the entries in the matrix $\mathbf{M}$, whose $\mathbf{RM}$ will give this number?

The answer is as follows: When the $\mathbf{RD}_e$ matrix is used instead of $\mathbf{D}_e$, the W index has to be changed with the Harary number, H_{De}, and the resulting number, called H_{Tr}, is a Harary-type one. We call it a "hyper-Harary analogue" since it obeys a relation formally identical to eq **6**

$$H_{Tr} = (\mathrm{Tr}(\mathbf{RD}_e^2)/2 + H_{De})/2 \qquad (10)$$

However, the matrix $\mathbf{M} = \mathbf{D}_{Tr}$ (see eqs **7, 8** and Figure **1**), whose $\mathbf{RM}$ gives the number H_{Tr},, is not a path defined one. This matrix is a fiction, devised only for the symmetry of relations **(6)** and **(9)**. The two hyper-Harary indices, H_{Dp} and H_{Tr}, are highly intercorrelated (within the set of octanes), as can be seen from the subsequent intercorrelating matrix.

Intercorrelating matrix of Harary-type indices in octanes

	H_{De}	H_{Dp}	H_{Tr}
H_{De}	**1**	**0.9989**	**0.9996**
H_{Dp}		**1**	**0.9998**
H_{Tr}			**1**

Harary-type numbers for nonanes are listed in Table **1**.

Table 1. Harary-type indices of the matrices $\mathbb{RD}_e$, $\mathbb{RD}_p$ and $\mathbb{RD}_{Tr}$ of nonanes

Graph	H_{De}	H_{Dp}	H_{Tr}
nonane	16.46071	12.34206	13.74483
2-methyloctane	16.83571	12.64762	14.04952
3-methyloctane	17.02619	12.77857	14.19010
4-methyloctane	17.10952	12.83095	14.24913
3-ethylheptane	17.30000	12.96190	14.38972
4-ethylheptane	17.38333	13.01429	14.44875
2,2-dimethylheptane	17.55000	13.24286	14.63625
2,3-dimethylheptane	17.55000	13.19524	14.60847
2,4-dimethylheptane	17.51667	13.16190	14.57875
2,5-dimethylheptane	17.41667	13.09524	14.50625
2,6-dimethylheptane	17.21667	12.95714	14.35847
3,3-dimethylheptane	17.88333	13.48095	14.88625
3,4-dimethylheptane	17.76667	13.34762	14.76972
3,5-dimethylheptane	17.63333	13.24762	14.66750
4,4-dimethylheptane	17.98333	13.54762	14.95875
3-ethyl-2-methylhexane	17.85000	13.40000	14.82875
3-ethyl-3-methylhexane	18.23333	13.73333	15.14972
3-ethyl-4-methylhexane	17.98333	13.50000	14.93097
4-ethyl-2-methylhexane	17.71667	13.30000	14.72653
2,2,3-trimethylhexane	18.35000	13.86667	15.26625
2,2,4-trimethylhexane	18.18333	13.73333	15.13431
2,2,5-trimethylhexane	17.95000	13.56667	14.95958
2,3,3-trimethylhexane	18.48333	13.96667	15.36847
2,3,4-trimethylhexane	18.23333	13.73333	15.14972
2,3,5-trimethylhexane	17.96667	13.53333	14.94528
2,4,4-trimethylhexane	18.31667	13.83333	15.23653
3,3,4-trimethylhexane	18.61667	14.06667	15.47069
3,3-diethylpentane	18.50000	13.93333	15.35417
2,2-dimethyl-3-ethylpentane	18.58333	14.03333	15.44097
2,3-dimethyl-3-ethylpentane	18.75000	14.16667	15.57292
2,4-dimethyl-3-ethylpentane	18.33333	13.80000	15.22222
2,2,3,3-tetramethylpentane	19.25000	14.63333	16.01042
2,2,3,4-tetramethylpentane	18.83333	14.26667	15.65972
2,2,4,4-tetramethylpentane	18.75000	14.23333	15.61458
2,3,3,4-tetramethylpentane	19.00000	14.40000	15.79167

Polynomials of reciprocal distance matrices

The polynomial $\mathbf{RD_e(G,x)}$ of a graph G is the characteristic polynomial of the $\mathbb{RD}_e$ matrix[2,3,20]

$$\mathbf{RD_e(G,x) = det\ (xI - \mathbb{RD}_e)} \qquad (11)$$

A list of $\mathbf{RD_e(G,x)}$ polynomials for a collection of path- ($\mathbf{L_N}$) and cyclic-graphs ($\mathbf{C_N}$) (with $\mathbf{N}$ = 2 to 10) is presented in the following.

$\mathbf{RD_e(L_2) = x^2 - 1}$

$\mathbf{RD_e(L_3) = x^3 - 2.25000x - 1}$

$\mathbf{RD_e(L_4) = x^4 - 3.61111x^2 - 2.66667x - 0.15972}$

$\mathbf{RD_e(L_5) = x^5 - 5.03472x^3 - 4.79167x^2 - 0.11092x + 0.61227}$

$\mathbf{RD_e(L_6) = x^6 - 6.49833x^4 - 7.25000x^3 + 0.52844x^2 + 2.88479x + 0.64451}$

$\mathbf{RD_e(L_7) = x^7 - 7.98972x^5 - 9.96204x^4 + 2.07622x^3 + 7.94928x^2 + 2.97405x + 0.06688}$

$\mathbf{RD_e(L_8) = x^8 -9.50152x^6 -12.87407x^5 +4.78665x^4 +16.87871x^3 +8.06698x^2 -0.11232x - 0.46868}$

$\mathbf{RD_e(L_9) = x^9 - 11.02894x^7 - 15.94816x^6 + 8.86287x^5 + 30.64313x^4 + 16.81716x^3}$
$\mathbf{- 1.74388x^2 - 3.18855x - 0.48358}$

$\mathbf{RD_e(L_{10}) = x^{10} - 12.56871x^8 - 19.15647x^7 + 14.46873x^6 + 50.10378x^5 + 29.82450x^4}$
$\mathbf{- 7.30498x^3 - 12.08817x^2 - 3.07542x - 0.06892}$

$\mathbf{RD_e(C_3) = x^3 - 3x - 2}$

$\mathbf{RD_e(C_4) = x^4 - 4.50000x^2 - 4.50000x - 0.93750}$

$\mathbf{RD_e(C5) = x^5 - 6.25000x^3 - 7.50000x^2 - 2.18750x - 0.18750}$

$\mathbf{RD_e(C_6) = x^6 - 7.83333x^4 - 10.50000x^3 - 1.90046x^2 + 1.65278x - 0.16804}$

$\mathbf{RD_e(C_7) = x^7 - 9.52778x^5 - 14.38889x^4 - 1.73920x^3 + 6.45988x^2 + 1.33936x - 1.00351}$

$\mathbf{RD_e(C_8) = x^8 - 11.13889x^6 - 17.88889x^5 + 0.91387x^4 + 17.06327x^3 + 6.45222x^2 - 4.06499x - 2.13145}$

$\mathbf{RD_e(C_9) = x^9 - 12.81250x^7 - 21.97222x^6 + 3.95443x^5 + 32.58174x^4 + 16.85838x^3}$
$\mathbf{- 9.30651x^2 - 9.86337x - 2.16958}$

$\mathbf{RD_e(C_{10}) = x^{10} - 14.43611x^8 - 25.76389x^7 + 9.80588x^6 + 56.47785x^5 + 34.10229x^4}$
$\mathbf{- 20.69571x^3 - 30.94614x^2 - 12.05529x - 1.56442}$

The spectrum **Sp(RD$_e$,G)** represents the eigenvalues of the matrix **$\mathbb{RD}_e$(G)** (or the solutions of **RD$_e$(G,x)** polynomial). For the above collection of graphs, the spectrum is given in Appendix. ***MaxSp*($\mathbb{RD}_e$,G)** and ***MinSp*($\mathbb{RD}_e$,G)** values, for nonanes, are given in Table **2**.

The polynomial **RD$_e$(G,x)** is the first representant of polynomials with real number coefficients. The coefficients of **RD$_e$(G,x)** are appropriate for building a ***Z*** index[16] analogue, by summing their absolute values (in the opposite to the values of **D$_e$(G,x)**, which are too large)

$$SumCh(\mathbb{RD}_e) = \sum_k \left| a_k(\mathbf{RD}_e(G,x)) \right| \qquad (12)$$

Values of this index for nonanes are given in Table **3**.

The polynomial **RD$_p$(G,x)** of a graph **G** is the characteristic polynomial of the matrix $\mathbb{RD}_p$

$$\mathbf{RD}_p(G,x) = \det(xI - \mathbb{RD}_p) \qquad (13)$$

This is another polynomial with real number coefficients. They are also good for devising a ***SumCh*($\mathbb{RD}_p$)** descriptor, according to eq **12**. Values of this index for nonanes are given in Table **3**.

RD$_p$(G,x) polynomials for the above collection of graphs are listed in the following.

$\mathbf{RD}_p(L_2) = x^2 - 1$

$\mathbf{RD}_p(L_3) = x^3 - 2.11111x - 0.66667$

$\mathbf{RD}_p(L_4) = x^4 - 3.25x^2 - 1.55556x + 0.44753$

$\mathbf{RD}_p(L_5) = x^5 - 4.39889x^3 - 2.53333x^2 + 1.79164x + 0.84720$

$\mathbf{RD}_p(L_6) = x^6 - 5.55222x^4 - 3.55259x^3 + 4.24793x^2 + 3.20421x + 0.11116$

$\mathbf{RD}_p(L_7) = x^7 - 6.70782x^5 - 4.59355x^4 + 7.91997x^3 + 7.46495x^2 + 0.01529x - 0.69143$

$\mathbf{RD}_p(L_8) = x^8 - 7.86470x^6 - 5.646856x^5 + 12.86059x^4 + 13.85582x^3 - 1.029420x^2 - 3.72491x - 0.52987$

$\mathbf{RD}_p(L_9) = x^9 - 9.02235x^7 - 6.70769x^6 + 19.09852x^5 + 22.50937x^4 - 4.05915x^3 - 11.57102x^2$
$- 2.55160x + 0.28197$

$\mathbf{RD}_p(L_{10}) = x^{10} - 10.18049x^8 - 7.77335x^7 + 26.65027x^6 + 33.50570x^5 - 10.29718x^4$
$- 27.29578x^3 - 7.02623x^2 + 2.35164x + 0.63848$

$RD_p(C_3) = x^3 - 3x - 2$

$RD_p(C_4) = x^4 - 4.22222x^2 - 2.66667x - 0.43210$

$RD_p(C_5) = x^5 - 5.55556x^3 - 4.44444x^2 + 0.80247x - 0.03292$

$RD_p(C_6) = x^6 - 6.75000x^4 - 5.48148x^3 + 4.44676x^2 + 2.85185x - 1.446181$

$RD_p(C_7) = x^7 - 7.97222x^5 - 6.87037x^4 + 8.80401x^3 + 8.86523x^2 - 2.62755x - 2.86272$

$RD_p(C_8) = x^8 - 9.15111x^6 - 7.97037x^5 + 15.21332x^4 + 18.37315x^3 - 4.38180x^2 - 10.54136x - 2.96519$

$RD_p(C_9) = x^9 - 10.34000x^7 - 9.20778x^6 + 22.57359x^5 + 30.34146x^4 - 7.43043x^3 - 24.25741x^2 - 10.14790x - 1.24871$

$RD_p(C_{10}) = x^{10} - 11.51111x^8 - 10.31481x^7 + 31.66023x^6 + 45.48037x^5 - 13.91700x^4 - 49.06050x^3 - 23.45637x^2 - 2.37437x - 0.06850$

The spectrum **Sp(RD$_p$,G)** represents the eigenvalues of the matrix **RD$_p$(G)** (or the zeros of **RD$_p$(G,x)** polynomial). For the above collection of graphs, the spectrum is given in Appendix. ***MaxSp*(RD$_p$,G)** and ***MinSp*(RD$_p$,G)** values, for nonanes, are given in Table **2**.

Table 2. Spectral maximum- and minimum-values, *MaxSp(M)* and *MinSp(M)* for matrices RD$_e$, RD$_p$ and RD$_{Tr}$ of nonanes

Graph	*MaxSp*(RD$_e$)	*MinSp*(RD$_e$)	*MaxSp*(RD$_p$)	*MinSp*(RD$_p$)	*MaxSp*(RD$_{Tr}$)	*MinSp*(RD$_{Tr}$)
nonane	3.74049	-1.35934	2.86405	-1.50438	3.15196	-1.47616
2-methyloctane	3.83088	-1.37996	2.95005	-1.53602	3.23497	-1.50436
3-methyloctane	3.88949	-1.39550	3.00846	-1.55719	3.28846	-1.52493
4-methyloctane	3.91810	-1.39977	3.03669	-1.56405	3.31421	-1.53120
3-ethylheptane	3.97103	-1.41138	3.08549	-1.57901	3.36086	-1.54639
4-ethylheptane	3.99693	-1.41380	3.10919	-1.58341	3.38340	-1.55020
2,2-dimethylheptane	4.01806	-1.42805	3.14395	-1.61411	3.41363	-1.57220
2,3-dimethylheptane	4.02525	-1.42656	3.14098	- 1.60122	3.41348	-1.56695
2,4-dimethylheptane	4.01378	-1.41047	3.12405	- 1.58370	3.40025	-1.54769
2,5-dimethylheptane	3.97924	-1.40690	3.08773	- 1.57368	3.36817	-1.54096
2,6-dimethylheptane	3.91897	-1.38971	3.02879	- 1.55314	3.31370	-1.51907
3,3-dimethylheptane	4.11610	-1.44856	3.23864	- 1.63937	3.50231	-1.59914

Table 2. (continued):

3,4-dimethylheptane	4.08704	-1.43564	3.19876	- 1.61449	3.46844	-1.57975
3,5-dimethylheptane	4.04390	-1.41791	3.15142	- 1.59188	3.42693	-1.55703
4,4-dimethylheptane	4.14666	-1.44904	3.26671	- 1.64242	3.52914	-1.60085
3-ethyl-2-methylhexane	4.11002	-1.43757	3.21809	- 1.61754	3.48758	-1.58262
3-ethyl-3-methylhexane	4.21215	-1.46425	3.32759	-1.66013	3.58753	-1.62037
3-ethyl-4-methylhexane	4.14491	-1.44343	3.25077	-1.62582	3.51890	-1.59070
4-ethyl-2-methylhexane	4.06796	-1.42181	3.17265	-1.59690	3.44738	-1.56218
2,2,3-trimethylhexane	4.22683	-1.46809	3.34175	-1.66547	3.60252	-1.62552
2,2,4-trimethylhexane	4.17365	-1.44043	3.28144	-1.63412	3.55010	-1.59116
2,2,5-trimethylhexane	4.10574	-1.43649	3.21592	-1.62286	3.48894	-1.58317
2,3,3-trimethylhexane	4.26454	-1.47565	3.37855	-1.67556	3.63697	-1.63570
2,3,4-trimethylhexane	4.19587	-1.45225	3.29952	-1.63949	3.56682	-1.60322
2,3,5-trimethylhexane	4.11950	-1.43469	3.22289	-1.61458	3.49631	-1.57927
2,4,4-trimethylhexane	4.21307	-1.45241	3.32182	-1.64899	3.58686	-1.60653
3,3,4-trimethylhexane	4.29734	-1.47908	3.40732	-1.68051	3.66544	-1.64063
3,3-diethylpentane	4.28067	-1.47715	3.39074	-1.67632	3.64837	-1.63745
2,2-dimethyl-3-ethylpentane	4.28732	-1.47211	3.39470	-1.67303	3.65463	-1.63200
2,3-dimethyl-3-ethylpentane	4.33247	-1.48654	3.44033	-1.68978	3.69687	-1.65043
2,4-dimethyl-3-ethylpentane	4.22361	-1.45385	3.32419	-1.64346	3.59063	-1.60609
2,2,3,3-tetramethylpentane	4.44311	-1.50871	3.55113	-1.72322	3.80257	-1.68166
2,2,3,4-tetramethylpentane	4.33528	-1.47691	3.43782	-1.68096	3.69838	-1.63923
2,2,4,4-tetramethylpentane	4.30235	-1.45211	3.40460	-1.66039	3.66943	-1.61120
2,3,3,4-tetramethylpentane	4.38245	-1.49436	3.48702	-1.70125	3.74311	-1.66141

Table 3. ***SumCh*(𝕄) indices of the matrices $\mathbb{RD}_e$, $\mathbb{RD}_p$ and $\mathbb{RD}_{Tr}$ of nonanes**

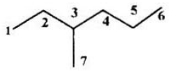
Graph	*SumCh*($\mathbb{RD}_e$)	*SumCh*($\mathbb{RD}_p$)	*SumCh*($\mathbb{RD}_{Tr}$)
nonane	89.71628	76.80166	74.47887
2-methyloctane	93.88263	72.45017	76.99909
3-methyloctane	85.31952	66.37881	70.74557
4-methyloctane	78.07320	69.57511	70.42638
3-ethylheptane	69.78597	65.63738	64.46931
4-ethylheptane	67.74463	69.21294	63.70341
2,2-dimethylheptane	96.32293	71.21244	73.49137
2,3-dimethylheptane	79.90156	65.35204	68.02870
2,4-dimethylheptane	79.57659	69.41800	71.31552
2,5-dimethylheptane	90.35920	68.49660	71.52305
2,6-dimethylheptane	101.00045	74.19637	77.37119
3,3-dimethylheptane	80.88253	62.36811	64.07756
3,4-dimethylheptane	72.26710	60.10992	62.19378
3,5-dimethylheptane	78.56807	63.31859	65.74621
4,4-dimethylheptane	73.40243	63.28952	63.87003
3-ethyl-2-methylhexane	68.47534	62.61426	61.82100
3-ethyl-3-methylhexane	67.15264	54.60532	54.77622
3-ethyl-4-methylhexane	65.11322	58.30437	56.59608
4-ethyl-2-methylhexane	73.47414	63.59971	65.32280
2,2,3-trimethylhexane	83.51070	61.19526	61.09192
2,2,4-trimethylhexane	93.75835	66.38074	70.16383
2,2,5-trimethylhexane	107.81940	75.70775	81.15811
2,3,3-trimethylhexane	76.32096	58.05071	57.59757
2,3,4-trimethylhexane	76.90603	58.24704	58.95942
2,3,5-trimethylhexane	87.20227	66.55531	67.41497
2,4,4-trimethylhexane	85.75659	63.07368	63.60943
3,3,4-trimethylhexane	73.21446	52.94883	52.67924
3,3-diethylpentane	61.26824	53.04559	46.46048
2,2-dimethyl-3-ethylpentane	72.46244	56.75668	55.79395
2,3-dimethyl-3-ethylpentane	67.05941	49.70956	49.12687
2,4-dimethyl-3-ethylpentane	69.86495	58.96288	58.61520
2,2,3,3-tetramethylpentane	77.44882	50.00178	49.85732
2,2,3,4-tetramethylpentane	86.60200	58.77651	60.13555
2,2,4,4-tetramethylpentane	108.76769	78.82451	80.42922
2,3,3,4-tetramethylpentane	76.27681	52.44864	50.79866

The polynomial $\mathbf{RD}_{Tr}(\mathbf{G},x)$ of a graph **G** is the characteristic polynomial of the matrix $\mathbb{RD}_{Tr}$

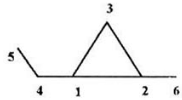
$$\mathbf{RD}_{Tr}(\mathbf{G},x) = \det(x\mathbf{I} - \mathbb{RD}_{Tr}) \qquad (14)$$

This is a third polynomial with real number coefficients. They are also good for devising a ***SumCh***($\mathbb{RD}_{Tr}$) descriptor, according to eq **12**. Values of this index for nonanes are given in Table **3**. Figure **2** illustrates the $\mathbf{RD}_{Tr}$ matrix, polynomial and corresponding spectral data for the graphs 3-methylhexane, **2** and 1-ethyl-2-methylcyclopropane, **3**.

Figure 2. $\mathbb{RD}_{Tr}$ matrix, its characteristic polynomials and spectrum for the graphs: 3-methylhexane, 2 and 1-ethyl-2-methylcyclopropane, 3



2



3

$\mathbb{RD}_{Tr}$**(2)**

0.00000	1.00000	0.37500	0.22222	0.15625	0.12000	0.22222
1.00000	0.00000	1.00000	0.37500	0.22222	0.15625	0.37500
0.37500	1.00000	0.00000	1.00000	0.37500	0.22222	1.00000
0.22222	0.37500	1.00000	0.00000	1.00000	0.37500	0.37500
0.15625	0.22222	0.37500	1.00000	0.00000	1.00000	0.22222
0.12000	0.15625	0.22222	0.37500	1.00000	0.00000	0.15625
0.22222	0.37500	1.00000	0.37500	0.22222	0.15625	0.00000

Ch($\mathbb{RD}_{Tr}$, 2): $x^7 - 7.17831x^6 - 7.05179x^4 + 3.95220x^3 + 5.84156x^2 + 0.80096x - 0.28000$

SumCh($\mathbb{RD}_{Tr}$, **2**): = 26.10482

Sp($\mathbb{RD}_{Tr}$, 2): {2.97832, 0.88193, 0.15698, - 0.42674, - 0.87414, - 1.20273, - 1.51362}

$\mathbb{RD}_{Tr}$**(3)**

0.00000	1.00000	1.00000	1.00000	0.37500	0.37500
1.00000	0.00000	1.00000	0.37500	0.22222	1.00000
1.00000	1.00000	0.00000	0.37500	0.22222	0.37500
1.00000	0.37500	0.37500	0.00000	1.00000	0.22222
0.37500	0.22222	0.22222	1.00000	0.00000	0.15625
0.37500	1.00000	0.37500	0.22222	0.15625	0.00000

Figure 2. (continued):

Ch(ℝ𝔻$_{Tr}$, 3): $= x^6 - 6.87569x^4 - 7.68264x^3 + 0.74944x^2 + 2.99831x + 0.52642$

***SumCh*(ℝ𝔻$_{Tr}$, 3):** $= 19.83251$

Sp(ℝ𝔻$_{Tr}$, 3): {3.03515, 0.60903, - 0.20367, - 0.81615, - 1.21969, - 1.40468}

RD$_{Tr}$(G,x) polynomials for the above collection of graphs are listed in the following.

$Ch(RD_{Tr},L_2) = x^2 - 1$

$Ch(RD_{Tr},L_3) = x^3 - 2.14062x - 0.75000$

$Ch(RD_{Tr},L_4) = x^4 - 3.33063x^2 - 1.83333x + 0.28096$

$Ch(RD_{Tr},L_5) = x^5 - 4.54505x^3 - 3.09950x^2 + 1.27857x + 0.77328$

$Ch(RD_{Tr},L_6) = x^6 - 5.77388x^4 - 4.48067x^3 + 3.26057x^2 + 3.10271x + 0.25390$

$Ch(RD_{Tr},L_7) = x^7 - 7.01215x^5 - 5.94089x^4 + 6.39289x^3 + 7.59276x^2 + 0.81774x - 0.49147$

$Ch(RD_{Tr},L_8) = x^8 - 8.25709x^6 - 7.45889x^5 + 10.78416x^4 + 14.69528x^3 + 1.41323x^2 - 2.81469x - 0.54990$

$Ch(RD_{Tr},L_9) = x^9 - 9.50697x^7 - 9.02104x^6 + 16.50929x^5 + 24.75190x^4 + 1.44823x3$

$- 9.24505x^2 - 2.96463x + 0.03175$

$Ch(RD_{Tr},L_{10}) = x^{10} - 10.76066x^8 - 10.61807x^7 + 23.62222x^6 + 38.02639x^5 + 0.07153x^4$

$- 22.93163x^3 - 9.23432x^2 + 0.69254x + 0.46693$

$Ch(RD_{Tr},C_3) = x^3 - 3x - 2$

$Ch(RD_{Tr},C_4) = x^4 - 4.28125x^2 - 3x - 0.54272$

$Ch(RD_{Tr},C_5) = x^5 - 5.70312x^3 - 5.15625x^2 + 0.11841x - 0.00067$

$Ch(RD_{Tr},C_6) = x^6 - 6.99190x^4 - 6.71094x^3 + 2.86238x^2 + 2.72421x - 0.94336$

$Ch(RD_{Tr},C_7) = x^7 - 8.33005x^5 - 8.71219x^4 + 6.19238x^3 + 8.57656x^2 - 1.10111x - 2.15744$

$Ch(RD_{Tr},C_8) = x^8 - 9.61772x^6 - 10.42564x^5 + 11.63470x^4 + 18.50412x^3 - 0.63373x^2 - 8.15286x -2.55346$

$Ch(RD_{Tr},C_9) = x^9 - 10.92980x^7 - 12.36955x^6 + 17.99531x^5 + 31.69482x^4 + 0.29201x3$

$- 19.25122x^2 - 9.63591x - 1.36765$

$Ch(RD_{Tr},C_{10}) = x^{10} - 12.21622x^8 -14.14910x^7 + 26.33918x^6 + 49.36144x^5 + 0.31204x4$

$- 40.48124x^3 -25.01248x^2 -4.54703x -0.25576$

The spectrum $\mathbf{Sp}(\mathbb{RD}_{Tr},\mathbf{G})$ represents the eigenvalues of the matrix $\mathbb{RD}_{Tr}(\mathbf{G})$ (or the zeros of $\mathbf{RD}_{Tr}(\mathbf{G,x})$ polynomial). For the above collection of graphs, the spectrum is given in Appendix. $\boldsymbol{MaxSp}(\mathbb{RD}_{Tr},\mathbf{G})$ and $\boldsymbol{MinSp}(\mathbb{RD}_{Tr},\mathbf{G})$ values, for nonanes, are given in Table **2**.

Polynomials were calculated by the LeVerier-Frame-Fadeev method[21,22] implemented in an original program. Molecular graphs were introduced by HyperChem (4.5) program.

Correlating and separating tests

The newly resulting indices were tested for correlation with some physico-chemical properties of nonanes, listed in ref. 23: boiling point, BP, heat of vaporization, HV, molar refraction, MR, Molar volume, MV, critical pressure, CP, surface tension, ST and critical temperature, CT.

In *single variable regression*, none of the spectral data correlate satisfactorily. Maximum correlations are: BP, 0.580 with $\boldsymbol{SumCh}(\mathbb{RD}_e)$; HV, 0.698 with $\boldsymbol{MaxSp}(\mathbb{RD}_{Tr})$; MR, 0.953 with $\boldsymbol{SumCh}(\mathbb{RD}_{Tr})$; MV, 0.952 with $\boldsymbol{SumCh}(\mathbb{RD}_{Tr})$; CP, 0.840 with $\boldsymbol{SumCh}(\mathbb{RD}_{Tr})$; ST, 0.843 with $\boldsymbol{SumCh}(\mathbb{RD}_e)$ and TC, 0.834 with $\boldsymbol{SumCh}(\mathbb{RD}_{Tr})$.

Since the spectral descriptors are highly intercorrelated, except the $\boldsymbol{SumCh}(\mathbb{M})$, and no satisfactory correlation was found by using only spectral data, we introduced the walk numbers ${}^{e}W_A$. They are the classical molecular walk counts[24] of length **e** and can be defined[25] as

$$ {}^{e}W_A = (1/2)\sum_i {}^{e}W_{A,i} = (1/2)\sum_i \sum_j [\mathbf{A}^e]_{ij} \qquad \mathbf{(15)} $$

where ${}^{e}W_{A,i}$ is the row sum in the adjacency matrix raised at the power **e**. Table **4** lists ${}^{e}W_A$ values for nonanes.

In *three variable regression*, the best correlations obtained are: BP, r = 0.962; s = 1.726, with $\boldsymbol{MaxSp}(\mathbb{RD}_{Tr})$, $\mathbf{1/(^2}W_A\mathbf{)}$ and ${}^{7}W_A$; HV, r = 0.979; s = 0.343, with $\boldsymbol{MaxSp}(\mathbb{RD}_{Tr})$,

$1/({}^2W_A)$ and **${}^5W_A$**; MR, r = 0.965; s = 0.067, with ***Sum(***$\mathbb{RD}_{Tr}$**)**, **$1/({}^2W_A)$** and **${}^3W_A$** ; MV, r = 0.992; s = 0.421, with ***MaxSp(***$\mathbb{RD}_{Tr}$**)**, **$1/({}^2W_A)$** and **${}^3W_A$**; CP, 0.912; s = 0.589, with ***Sum(***$\mathbb{RD}_{Tr}$**)**, **$1/({}^2W_A)$** and **${}^3W_A$**; ST, r = 0.975; s = 0.227, with ***MaxSp(***$\mathbb{RD}_{Tr}$**)**, **$1/({}^2W_A)$** and **${}^7W_A$**; and CT, r = 0.917; s = 4.60, with ***Sum(***$\mathbb{RD}_{Tr}$**)**, **$1/({}^2W_A)$** and **${}^7W_A$**.

It is obvious that the walk numbers, (e.g. ${}^2W_A$ (as **$1/({}^2W_A)$**) and ${}^7W_A$) account for the majority of correlation: BP, 0.933; HV, 0.976; MR, 0.936; MV, 0.9758 CP, 0.906; ST, 0.973 and CT, 0.916.

Table 4. Walk numbers, 2^eW_A , of nonanes

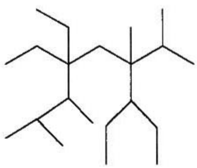
Graph	${}^1W_A$	${}^2W_A$	${}^3W_A$	${}^4W_A$	${}^5W_A$	${}^6W_A$	${}^7W_A$	${}^8W_A$
nonane	16	30	56	106	200	380	720	1370
2-methyloctane	16	32	60	120	228	456	872	1742
3-methyloctane	16	32	62	124	244	490	968	1948
4-methyloctane	16	32	62	126	248	506	1002	2046
3-ethylheptane	16	32	64	130	264	538	1096	2236
4-ethylheptane	16	32	64	132	268	554	1128	2332
2,2-dimethylheptane	16	36	68	154	296	674	1304	2980
2,3-dimethylheptane	16	34	68	142	292	608	1260	2624
2,4-dimethylheptane	16	34	66	124	278	600	1178	2544
2,5-dimethylheptane	16	34	66	138	274	568	1138	2346
2,6-dimethylheptane	16	34	64	134	256	534	1024	2134
3,3-dimethylheptane	16	36	72	162	332	748	1544	3482
3,4-dimethylheptane	16	34	70	148	310	656	1380	2920
3,5-dimethylheptane	16	34	68	144	292	618	1256	2658
4,4-dimethylheptane	16	36	72	166	336	780	1584	3684
3-ethyl-2-methylhexane	16	34	70	150	314	670	1410	3002
3-ethyl-3-methylhexane	16	36	76	172	368	834	1788	4054
3-ethyl-4-methylhexane	16	34	72	154	328	702	1496	3202
4-ethyl-2-methylhexane	16	34	68	146	296	632	1288	2788
2,2,3-trimethylhexane	16	38	78	180	382	872	1874	4258
2,2,4-trimethylhexane	16	38	74	176	346	822	1622	3850
2,2,5-trimethylhexane	16	38	72	168	328	752	1496	3388
2,3,3-trimethylhexane	16	38	80	184	400	912	2000	4548
2,3,4-trimethylhexane	16	36	76	166	356	776	1668	3634
2,3,5-trimethylhexane	16	36	72	158	324	702	1456	3132

Table 4 (continued):

2,4,4-trimethylhexane	16	38	76	180	364	862	1748	4148
3,3,4-trimethylhexane	16	38	82	188	414	946	2090	4772
3,3-diethylpentane	16	36	80	180	400	900	2000	4500
2,2-dimethyl-3-ethylpentane	16	38	80	188	400	936	2000	4672
2,3-dimethyl-3-ethylpentane	16	38	84	192	432	982	2216	5030
2,4-dimethyl-3-ethylpentane	16	36	76	170	360	840	1704	3804
2,2,3,3-tetramethylpentane	16	42	92	222	508	1200	2780	6522
2,2,3,4-tetramethylpentane	16	40	84	200	428	1014	2176	5152
2,2,4,4-tetramethylpentane	16	42	80	210	400	1050	2000	5250
2,3,3,4-tetramethylpentane	16	40	88	204	464	1064	2432	5568

***SumCh*(RM)** indices were successfully tested in discriminating a pair of graphs (**4**;**5** - Figures **3** and **4**) built up so that they show identical pairwise distance degree sequence, **DDS** (40, 58, 76, 78, 72, 56, 32, 8) and degeneracy of most indices based on the distance in a graph.[26] All these indices (**RM** = $\mathbf{RD_e}$, $\mathbf{RD_p}$ and $\mathbf{RD_{Tr}}$) differentiate between the two nonisomorphic graphs. Spectral data also differentiate the two structures.

Figure 3. Polynomials and spectral data for the graph 4



4

Ch($\mathbf{RD_e}$, 4): x^{21}-36.51653x^{19}-120.12986x^{18} + 12.37329x^{17} + 738.91042x^{16} + 1416.06399x^{15} +412.57178x^{14} -2020.97316x^{13} -2875.08393x^{12} -811.41414x^{11} +1485.06841x^{10} +1600.77627x^{9} + 475.93444x^{8} -156.50318x^{7} -134.97521x^{6}-15.75514x^{5} +9.13716x^{4} +2.28160x^{3} -0.16457x^{2} -0.06337x + 0.00138

***SumCh*($\mathbf{RD_e}$, 4)** = 12325.69784

Figure 3 (continued):

Sp(RD_e, 4): {7.11012, 2.47307, 1.13011, 0.99241, 0.30328, 0.30328, 0.18719, 0.01399, - 0.37566, - 0.50000, - 0.50000, - 0.57506, - 0.78956, - 0.98727, - 1.05328 - 1.05328, - 1.07165, - 1.28733, - 1.31371, - 1.47407, - 1.53757}

Ch(RD_p, 4): $x^{21} -24.91476x^{19} -36.44525x^{18} +165.27448x^{17} +427.89584x^{16} -172.10994x^{15} -1421.55537x^{14} -898.76328x^{13} +1583.62164x^{12} +2189.82758x^{11} -99.18743x^{10} -1511.61831x^{9} -589.48853x^{8} +368.92465x^{7} +284.84389x^{6} -3.40320x^{5} -45.68165x^{4} -9.12211x^{3} +1.75143x^{2} +0.71805x + 0.05864$

***SumCh*(RD_p, 4) =** 9836.20605

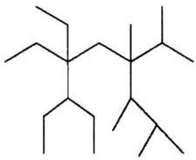
Sp(RD_p, 4): {4.69866, 2.70218, 1.50761, 1.37833, 0.62479, 0.62479, 0.50299, 0.32078, - 0.16008,- 0.33333, - 0.33333, - 0.41687, - 0.69002, - 0.96698, - 1.05813 - 1.05813, - 1.08608, - 1.39055, - 1.42917, - 1.66820, - 1.76927}

Ch(RD_{Tr}, 4): $x^{21} -27.81627x^{19} -56.21860x^{18} +137.39703x^{17} +532.57099x^{16} +203.71182x^{15} -1197.75594x^{14} -1592.75479x^{13}+386.89797x^{12}+2046.04204x^{11} +1023.58663x^{10} -655.83384x^{9} -740.32957x^{8} -49.67742x^{7} +171.78628x^{6} +53.00526x^{5} -12.35611x^{4} -7.44673x^{3} -0.32192x^{2} + 0.26565x + 0.03303$

***SumCh*(RD_{Tr}, 4) =** 8896.80789

Sp(RD_{Tr}, 4): {5.51173, 2.53077, 1.35648, 1.22743, 0.51981, 0.51981, 0.42862, 0.23644, - 0.20002, - 0.37500, - 0.37500, - 0.43696, - 0.69632, - 0.95769, - 1.05106, - 1.05106 - 1.06738, - 1.36354, - 1.39996, - 1.62952, - 1.72758}

Figure 4. Polynomials and spectral data for the graph 5



5

Ch(RD$_e$,5): x^{21} -36.51653x^{19} -120.12986x^{18} +12.36839x^{17} +738.83171x^{16} +1415.47877x^{15} +409.88866x^{14}-2029.49068x^{13} -2894.96606x^{12} -846.67574x^{11} + 1436.83721x^{10} +1549.92193x^{9} +435.46038x^{8} -179.30543x^{7} -142.28159x^{6} -15.32045x^{5} +10.78614x^{4} + 2.93053x^{3} -0.13309x^{2} -0.10443x -0.00660

***SumCh*(RD$_e$,5)** = 12278.43422

Sp(RD$_e$,5): {7.11017, 2.47568, 1.18486, 0.91996, 0.30328, 0.30328, 0.26637, - 0.09760, - 0.29003, - 0.50000, - 0.50000, - 0.61149, - 0.81708, - 0.92492, - 1.05328, - 1.05328, - 1.11283, - 1.26531, - 1.32654, - 1.47357, - 1.53768}

Ch(RD$_p$,5): x^{21} -24.91476x^{19} -36.44525x^{18} +165.27379x^{17} +427.88346x^{16} -172.21174x^{15} -1422.07236x^{14}-900.60094x^{13} +1578.76196x^{12} +2180.04064x^{11} -114.13614x^{10} -1528.28444x^{9} -601.21181x^{8} +367.66114x^{7} +292.64648x^{6} +5.22609x^{5} -42.52724x^{4} -10.08087x^{3} + 0.52669x^{2} +0.33450x + 0.01779

***SumCh*(RD$_p$,5)** = 9871.85809

Sp(RD$_p$,5): {4.69881, 2.69946, 1.56830, 1.29613, 0.62479, 0.62479, 0.60433, 0.18361, - 0.06666, - 0.33333, - 0.33333, - 0.44621, - 0.73230, - 0.88905, - 1.05813, - 1.05813, - 1.13915, - 1.35818, - 1.44900, - 1.66731, - 1.76943}

Figure 4 (continued):

Ch(RD$_{Tr}$,5): $x^{21} -27.81627x^{19} -56.21860x^{18} +137.39555x^{17} +532.54629x^{16} +203.52565x^{15}$
$-1198.60791x^{14} -1595.44385x^{13} +380.62709x^{12} +2034.87320x^{11} +1008.29337x^{10}$
$-671.68909x^{9} -752.02459x^{8} -54.13775x^{7} +173.89147x^{6} +57.38503x^{5}$
$-9.85728x^{4} -7.26482x^{3} -0.74621x^{2} + 0.08648x + 0.01056$

***SumCh*(RD$_{Tr}$,5)** = 8903.44108

Sp(RD$_{Tr}$,5): {5.51180, 2.52828, 1.41182, 1.15274, 0.51981, 0.51981, 0.51447, 0.11327,
- 0.10442, - 0.37500, - 0.37500, - 0.47311, - 0.73592, - 0.87749, - 1.05106,
- 1.05106, - 1.12095, - 1.33326, - 1.41824, - 1.62877, - 1.72773}

Conclusions

Matrices based on reciprocal distances in graph are useful descriptors for molecular structures. The Harary indices are obtained on these matrices by the Wiener operator (i.e. the half sum of the matrix entries). The Hyper-Harary analogue, H_{Tr}, and the corresponding matrix, **RD**$_{Tr}$, by means of spectral parameters, proved good correlating ability within the set of nonanes and good discriminating power. They are valuable partners in multivariate regression analysis and deserve further attention.

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Appendix

1. Spectra of $RD_e(G,x)$ polynomials in path graphs L_2 to L_{10} and cycles C_3 to C_{10}

$Sp(\mathbb{RD}_e, L_2)$ = {1.00000, -1.00000}

$Sp(\mathbb{RD}_e, L_3)$ = {1.68614, -0.50000, -1.18614}

$Sp(\mathbb{RD}_e, L_4)$ = {2.20326, -0.06574, -0.86992, -1.26759}

$Sp(\mathbb{RD}_e, L_5)$ = {2.61684, 0.30328, -0.56081, -1.05328, -1.30603}

$Sp(\mathbb{RD}_e, L_6)$ = {2.96093, 0.62047, -0.27855, -0.82466, -1.14905, -1.32914}

$Sp(\mathbb{RD}_e, L_7)$ = {3.25530, 0.89725, -0.02402, -0.60368, -0.97150, -1.21024, -1.34311}

$Sp(\mathbb{RD}_e, L_8)$ = {3.51238, 1.14216, 0.20578, -0.39636, -0.79270, -1.06925, -1.24927, -1.35275}

$Sp(\mathbb{RD}_e, L_9)$ = {3.74049, 1.36147, 0.41433, -0.20363, -0.61980, -0.92232, -1.13402, -1.27719, -1.35934

$Sp(\mathbb{RD}_e, L_{10})$ = {3.94547, 1.55986, 0.60477, -0.02479, -0.45534, -0.77653, -1.01068, -1.18159, -1.29692, -1.36425}

$Sp(\mathbb{RD}_e, C_3)$ = {2.00000, -1.00000, -1.00000}

$Sp(\mathbb{RD}_e, C_4)$ = {2.50000, -0.50000, -0.50000, -1.50000}

$Sp(\mathbb{RD}_e, C_5)$ = {3.00000, -0.19098, -0.19098, -1.30902, -1.30902}

$Sp(\mathbb{RD}_e, C_6)$ = {3.33333, 0.16667, 0.16667, -1.16667, -1.16667, -1.33333}

$Sp(\mathbb{RD}_e, C_7)$ = {3.66667, 0.42381, 0.42381, -0.93035, -0.93035, -1.32680, -1.32680}

$Sp(\mathbb{RD}_e, C_8)$ = {3.91667, 0.69281, 0.69281, -0.75000, -0.75000, -1.19281, -1.19281, -1.41667}

$Sp(\mathbb{RD}_e, C_9)$ = {4.16667, 0.90256, 0.90256, -0.54271, -0.54271, -1.08333, -1.08333, - 1.35985, -1.35985}

$Sp(\mathbb{RD}_e, C_{10})$ = {4.36667, 1.11653, 1.11653, -0.37582, -0.37582, -0.93320, -0.93320, -1.30751, -1.30751, -1.36667}

2. Spectra of $RD_p(G,x)$ polynomials in path graphs L_2 to L_{10} and cycles C_3 to C_{10}

$Sp(RD_p, L_2)$ = {1.00000, -1.00000}

$Sp(RD_p, L_3)$ = {1.59067, -0.33333, -1.25733}

$Sp(RD_p, L_4)$ = {1.98025, 0.20283, -0.81359, -1.36950}

$Sp(RD_p, L_5)$ = {2.25741, 0.62479, -0.39810, -1.05813, -1.42598}

$Sp(RD_p, L_6)$ = {2.46525, 0.96196, -0.03651, -0.73595, -1.19541, -1.45934}

$Sp(RD_p, L_7)$ = {2.62724, 1.23669, 0.27400, -0.43524, -0.94005, -1.28240, -1.48024}

$Sp(RD_p, L_8)$ = {2.75725, 1.46465, 0.54121, -0.16319, -0.68938, -1.07608, -1.34003, -1.49443}

$Sp(RD_p, L_9)$ = {2.86405, 1.65685, 0.77267, 0.08061, -0.45362, -0.86542, -1.16999, -1.38077, -1.50438

$Sp(RD_p, L_{10})$ = {2.95342, 1.82112, 0.97474, 0.29881, -0.23566, -0.66103, -0.99093, -1.23848, -1.41030, -1.51169}

$Sp(RD_p, C_3)$ = {2.00000, -1.00000, -1.00000}

$Sp(RD_p, C_4)$ = {2.33333, -0.33333, -0.33333, -1.66667}

$Sp(RD_p, C_5)$ = {2.66667, 0.07869, 0.07869, -1.41202, -1.41202}

$Sp(RD_p, C_6)$ = {2.83333, 0.50000, 0.50000, -1.16667, -1.16667, -1.50000}

$Sp(RD_p, C_7)$ = {3, 0.79831, 0.79831, -0.83786, -0.83786, -1.46045, -1.46045}

$Sp(RD_p, C_8)$ = {3.10000, 1.07851, 1.07851, -0.56667, -0.56667, -1.27851, -1.27851, -1.56667}

$Sp(RD_p, C_9)$ = {3.20000, 1.29325, 1.29325, -0.29262, -0.29262, -1.10000, -1.10000, -1.50063, -1.50063}

$Sp(RD_p, C_{10})$ = {3.26667, 1.49257, 1.49257, -0.06251, -0.06251, -0.89257, -0.89257, -1.40415, -1.40415, -1.53333}

3. Spectra of $RD_{Tr}(G,x)$ polynomials in path graphs, L_2-L_{10} and cycles C_3-C_{10}.

$Sp(RD_{Tr},L_2)$ = {1.00000, - 1.00000}

$Sp(RD_{Tr},L_3)$ = {1.61409, - 0.37500, - 1.23909}

$Sp(RD_{Tr},L_4)$ = {2.04005, 0.12500, - 0.81783, -1.34722}

$Sp(RD_{Tr},L_5)$ = {2.36008, 0.51981, - 0.42816, - 1.05106, - 1.40067}

$Sp(RD_{Tr},L_6)$ = {2.61375, 0.83849, - 0.09164, - 0.74776, - 1.17989, - 1.43295}

$Sp(RD_{Tr},L_7)$ = {2.82253, 1.10206, 0.19650, - 0.46717, - 0.93768, - 1.26336, - 1.45288}

$Sp(RD_{Tr},L_8)$ = {2.99923, 1.32479, 0.44471, - 0.21489, - 0.70206, - 1.06711, - 1.31802 - 1.46663}

$Sp(RD_{Tr},L_9)$ = {3.15196, 1.51643, 0.66064, 0.01037, - 0.48209, - 0.86832, -1.15557, - 1.35727, - 1.47616}

$Sp(RD_{Tr},L_{10})$ = {3.28621, 1.68385, 0.85044, 0.21175, - 0.27989, - 0.67682, - 0.98573, - 1.22112,
- 1.38545, - 1.48325}

$Sp(RD_{Tr},C_3)$ = {2.00000, - 1.00000, - 1.00000}

$Sp(RD_{Tr},C_4)$ = {2.37500, - 0.37500, - 0.37500, - 1.62500}

$Sp(RD_{Tr},C_5)$ = {2.75000, 0.01127, 0.01127, - 1.38627, - 1.38627}

$Sp(RD_{Tr},C_6)$ = {2.97222, 0.40278, 0.40278, - 1.15278, - 1.15278, - 1.47222}

$Sp(RD_{Tr},C_7)$ = {3.19444, 0.67966, 0.67966, - 0.84366, - 0.84366, - 1.43322, - 1.43322}

$Sp(RD_{Tr},C_8)$ = {3.35069, 0.94369, 0.94369, - 0.59375, - 0.59375, - 1.25619 - 1.25619 -1.53819}

$Sp(RD_{Tr},C_9)$ = {3.50694, 1.14645, 1.14645, - 0.34031, - 0.34031, - 1.08681- 1.08681, -1.47281 -1.47281}

$Sp(RD_{Tr},C_{10})$ = {3.62694, 1.33964, 1.33964, - 0.13172, - 0.13172, - 0.88867 - 0.88867, -1.38175,
-1.38175 -1.50194}

References

1. F. Harary, *Graph Theory*, Addison-Wesley, Reading, Ma, (1969).
2. O. Ivanciuc; T.S. Balaban; A.T. Balaban, Reciprocal Distance Matrix, Related Local Vertex Invariants and Topological Indices, *J.Math.Chem.* **12** (1993) 309-318
3. D. Plavšić; S. Nikolić; N. Trinajstić; Z. Mihalić, On the Harary Index for the Characterization of Chemical Graphs, *J.Math.Chem.* **12** (1993) 235-250.
4. H. Wiener, Structural Determination of Paraffin Boiling Points. *J.Am.Chem.Soc.* **69** (1947) 17-20
5. M.V. Diudea, Reciprocal Property or Harary Indices, *J.Chem.Inf.Comput.Sci.* (submitted)
6. M. Randić; X. Guo; T. Oxley; H. Krishnapriyan; L. Nayor, Wiener Matrix Invariants. *J Chem.Inf.Comput.Sci.* **34** (1994) 361-367.
7. M. Randić; X. Guo; T. Oxley; H. Krishnapriyan, Wiener Matrix: Source of Novel Graph Invariants, *J.Chem.Inf.Comput.Sci.* **33** (1993) 709-716
8. M.V. Diudea; O.M. Minailiuc; G. Katona; I. Gutman, Szeged Matrices and Related Numbers, *Commun.Math.Comput.Chem.* (*MATCH*), this issue.
9. M.V. Diudea; B. Pârv; M.I. Topan, Derived Szeged and Cluj Indices, *J.Serb.Chem.Soc.* **62** (1997) (in press).
10. M.V. Diudea, Cluj Matrix Invariants, *J.Chem.Inf.Comput.Sci.* (submitted).
11. M.V. Diudea, Cluj Matrix, CJ_u: Source of Various Graph Descriptors, *Commun.Math.Comput.Chem.* (*MATCH*), this issue.
12. M. Randić, Restricted Random Walks and Molecular Properties, *Theor.Chem.Acta* (in press).
13. O. Ivanciuc, Applications of Graph Theory in Organic Chemistry, Ph.D. Dissertation, Bucharest, (1996).
14. M.V. Diudea, Walk Numbers ^eW_M : Wiener-Type Numbers of Higher Rank, *J.Chem.Inf.Comput.Sci.* **36** (1996) 535-540.
15. M. Randić, Novel Molecular Descriptor for Structure-Property Studies, *Chem.Phys.Lett.* **211** (1993) 478-483.
16. H. Hosoya, Topological Index. A Newly Proposed Quantity Characterizing the Topological Nature of Structural Isomers of Saturated Hydrocarbons. *Bull.Chem.Soc Jpn.* **44** (1971) 2332-2339.

17. D.J. Klein; I. Lukovits; I. Gutman, On the Definition of the Hyper-Wiener Index for Cycle-Containing Structures. *J.Chem.Inf.Comput.Sci.* **35** (1995) 50-52.

18. M.V. Diudea; O. Ivanciuc, *Molecular Topology*, Comprex, Cluj, (1995).

19. M.V. Diudea, Wiener and Hyper-Wiener Numbers in a Single Matrix, *J. Chem.Inf.Comput.Sci.* **36** (1996) (in press).

20. O. Ivanciuc; M.V. Diudea, New Topological Matrices and Their Polynomials, *J. Chem.Inf. Comput. Sci.* (submitted).

21. K. Balasubramanian, Computer Generation of the Characteristic Polynomials of Chemical Graphs, *J.Comput.Chem.* **5** (1984) 387-394.

22. M. Barysz;. S. Nikolić; N. Trinajstić, A Note on the Characteristic Polynomial, *MATCH*, **19** (1986) 117-126.

23. D.E. Needham; I.C. Wei; P.G. Seybold, Molecular Modeling of the Physical Properties of the Alkanes, *J.Am.Chem.Soc.* **110** (1988) 4185-4194.

24. G. Rücker; Ch. Rücker, Counts of All Walks as Atomic and Molacular Descriptors, *J.Chem.Inf.Comput.Sci.* **33** (1993) 683-695.

25. M.V. Diudea; M. Topan; A. Graovac, A. Layer Matrices of Walk Degrees, *J.Chem.Inf Comput Sci.* **34** (1994) 1072-1078.

26. O. Ivanciuc; T.S. Balaban; A.T. Balaban, Chemical Graphs with Degenerate Topological Indices Based on Information on Distances, *J.Math.Chem.* **14** (1993) 21-33.