Indices of Reciprocal Properties or Harary Indices

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Reciprocal topological properties are used for building up novel indices referred to as Harary indices. They are defined by the aid of matrix algebra and examplified on appropriate sets of graphs. Analytical relations for calculating the indices, defined both on the basic and the reciprocal property, in particular classes of graphs are derived. The correlating and discriminating ability as well as the limitations of these indices are discussed.

INTRODUCTION

The earliest matrix representation of a graph, **G**, is by its adjacency matrix, A**(G)**, whose entries are unity, if any two vertices are adjacent (i.e., joined by an edge) and zero, otherwise. It was, probably, introduced by Sylvester,[1] in early 1870. Distance matrix, D**(G)**, having the entries equal to the number of edges between any two vertices, was introduced back in the 1960s, by Harary.[2]

In chemical graph theory, the distance matrix accounts for the "through bond" interactions of atoms in molecules. However, these interactions decrease as the distance between atoms increases. This is the reason why the groups of Balaban[3] and Trinajstić,[4−6] respectively, introduced, in 1993, the "reciprocal distance" matrix, RD**(G)**. Entries in this matrix are defined by

$$[\mathrm{RD}]_{ij} = 1/[\mathrm{D}]_{ij} \tag{1}$$

RD matrix allows the calculation of a Wiener index[7] analogue, as the half sum of its entries

$$H_D = (1/2)\sum_i\sum_j 1/[\mathrm{D}]_{ij} = (1/2)\sum_i\sum_j [\mathrm{RD}]_{ij} \tag{2}$$

The resulting number was called,[3,5] the "Harary index", in honor of Frank Harary. Since topological matrices are considered "natural" sources in deriving graph descriptors,[8,9] herein we investigate several matrices having entries as "reciprocal property".

NOVEL HARARY INDICES

Harary indices, H_M, are constructed, as an extension of the "reciprocal distance" index idea. Reciprocal matrices, RM, (i.e., matrices having $[\mathrm{RM}]_{ij} = 1/[\mathrm{M}]_{ij}$) are the ground of these indices

$$H_M = (1/2)\sum_i\sum_j 1/[\mathrm{M}]_{ij} = (1/2)\sum_i\sum_j [\mathrm{RM}]_{ij} \tag{3}$$

the subscript ***M*** being the identifier for the matrix M.

Distance matrix, and its reciprocal property matrix, will be marked, in the folowing, by $\mathrm{D_e}$ (i.e., distance-edge matrix) and $\mathrm{RD_e}$, for reasons detailed below.

Besides distance, four other topological properties (as entries in square matrices) are herein considered for evaluating their reciprocals:

Wiener matrix,[9] W, whose entries mean the number of "external" paths including a given path **(i,j),** and are calculated as the product

$$[\mathrm{W_{e/p}}]_{ij} = N_{i,e/p}\, N_{j,e/p} \tag{4}$$

where $N_{i,e/p}$ and $N_{j,e/p}$ denote the number of vertices (i.e., the cardinality of the set) lying on the two sides of the path **(i,j)**. Relation 4 is valid only in acyclic structures.

Note that the subscript **e/p** refers to the length of the path **(i,j)** on which the matrix is defined: **e** means a path equal to one edge (i.e., **(i,j)** ∈ **E(G)**, **E(G)** being the set of edges in graph), while **p** denotes a path of any length, one edge included (i.e., (i,j) ∈ **P(G)**, with **P(G)** the set of paths in graph). When the italicized symbol of a matrix is associated with the subscript **e**, it is an *index*, but it becomes a *hyper-index* (see below) when associated with a subscript **p**.

Szeged matrix,[10−16] SZ, whose entries denote the product of cardinalities of the sets $N_{i,e/p}$ and $N_{j,e/p}$, lying closer to the vertex **i** and **j**, respectively (the equidistant vertices not counted)

$$[\mathrm{SZ_{e/p}}]_{ij} = N_{i,e/p}\, N_{j,e/p} \tag{5}$$

$$N_{i,e/p} = |\{\mathbf{v}|\ \mathbf{v} \in \mathbf{V(G)};\quad [\mathrm{D_e}]_{iv} < [\mathrm{D_e}]_{jv}\}| \tag{6}$$

$$N_{j,e/p} = |\{\mathbf{v}\ |\mathbf{v} \in \mathbf{V(G)};\quad [\mathrm{D_e}]_{jv} < [\mathrm{D_e}]_{iv}\}| \tag{7}$$

Relations 5−7 are valid both for acyclic and cycle-containing graphs. $\mathrm{SZ_e}$ is identical to $\mathrm{W_e}$ in acyclic structures, but $\mathrm{SZ_p}$ is different from $\mathrm{W_p}$, both in acyclic and cycle containing graphs.

Cluj matrix,[17−19] CJ, whose entries collect the vertices lying closer to a focused vertex **i**, but out of the path **(i,j)** or, in other words, the "external" paths on the side of **i**, which include the path **(i,j)**. This matrix was built up according to the principle[20] of "single endpoint characterization of a path", thus resulting a square (in general), unsymmetric matrix, specified by a subscript **u**

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$$[CJ_u]_{ij} = N_{i,(i,j)} \tag{8}$$

$$N_{i,(i,j)} = \mathbf{max}|\{\mathbf{v}\,|\mathbf{v}\,|\mathbf{v} \in \mathbf{V(G)};\quad [D_e]_{iv} < [D_e]_{jv};\quad \mathbf{(i,v)}\cap\mathbf{(i,j)} = \mathbf{max}\{\mathbf{i}\};|\mathbf{(i,j)} = \mathbf{min}\}|$$

In that case when two or more paths **(i,j)** (i.e., two or more sets {**v**}) are encountered, the maximal cardinality of the sets {**v**} is taken, by definition. The relation 8 is valid both for acyclic and cyclic graphs. A symmetric Cluj matrix, $CJ_{e/p}$, was also derived[18] (see below). It is identical to the $W_{e/p}$ matrix in acyclic graphs but different in cycle-containing structures. CJ_e is identical to the SZ_e matrix, but CJ_p is different from SZ_p, in any graph. By analogy to CJ_u, an unsymmetric Szeged matrix was defined[16]

$$[SZ_u]_{ij} = N_{i,(i,j)} \tag{9}$$

$$N_{i,(i,j)} = \{\mathbf{v}\,|\mathbf{v} \in \mathbf{V(G)};\quad [D_e]_{iv} < [D_e]_{jv};|\mathbf{(i,j)}| = \mathbf{min}\}$$

SZ_u is a square (in general) unsymmetric matrix. The Cluj matrix, CJ_u, differs from SZ_u by the supplementary condition: $\mathbf{(i,v)}\cap\mathbf{(i,j)} = \mathbf{max}\{\mathbf{i}\}$.

Figure 1 illustrates the matrices D_e, SZ_u, and CJ_u and their reciprocal property matrices.

The M_u matrices (M being SZ and CJ) allow the construction of symmetric M_e and M_p matrices by relation

$$[M_{e/p}]_{ij} = [M_u]_{ij}\,[M_u]_{ji} \tag{10}$$

and the derivation of two Wiener-type indices, $\boldsymbol{I}$ (namely $\boldsymbol{M_e}$ or $\boldsymbol{M_p}$) by applying either the "Wiener operator" (i.e., the half sum of entries in a square matrix) on symmetric matrices

$$\boldsymbol{I} = (1/2)\sum_i\sum_j[M_{e/p}]_{ij} \tag{11}$$

or the so called[18] multiplicative "orthogonal operator" on unsymmetric matrices

$$\boldsymbol{I} = \sum_{(i,j)}[M_u]_{ij}[M_u]_{ji} \tag{12}$$

Walk matrix,[20] W, whose entries denote walks, starting from the focused vertex **i**, and having the length equal to the topological distance between **i** and any vertex **j** of a graph.

$$[W_{(A,D,1)}]_{ij} = {}^{[D]_{ij}}\boldsymbol{W}_{A,i}[\mathbf{1}]_{ij} \tag{13}$$

where **1** is the matrix with the off diagonal entries equal to 1. $W_{(A,D,1)}$ is a square (in general), unsymmetric matrix, and represents a particular case of the more general matrix, $W_{(M_1,M_2,M_3)}$.[20,21] $W_{(A,D,1)}$ and its reciprocal property matrix are examplified in Figure 2.

Wiener- and Harary-type indices herein discussed are examplified on a set of 30 cycloalkanes, in Table 1.

By virtue of the mutual relations between the basic properties, the Harary-type numbers show the following equalities: $\boldsymbol{H_{We}} = \boldsymbol{H_{SZe}} = \boldsymbol{H_{CJe}}$ (in trees) and $\boldsymbol{H_{SZe}} = \boldsymbol{H_{CJe}}$ (in any graph).

HYPER-HARARY NUMBERS

Randić has introduced[22] the notion of *hyper-index* in connection with the extension of the Wiener index/number

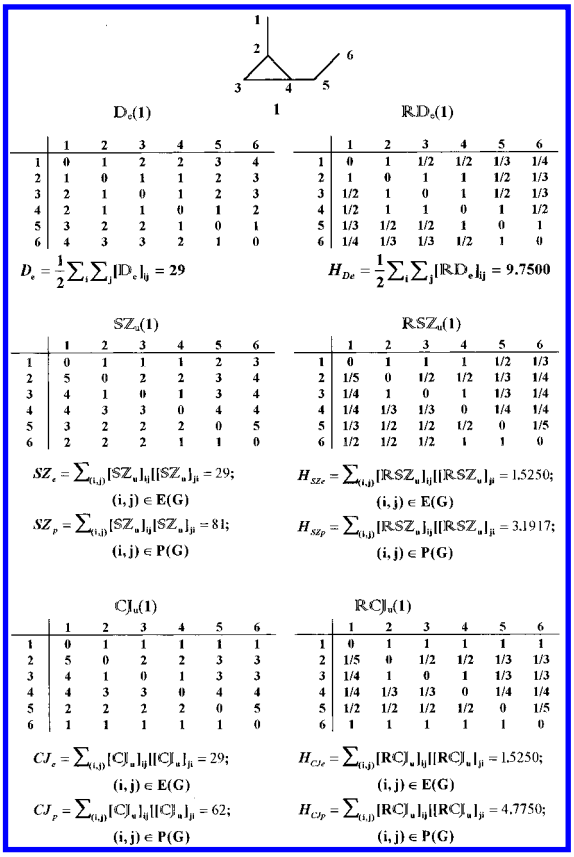


Figure 1. Matrices D_e, SZ_u, and CJ_u, their reciprocal property matrices, and corresponding indices.

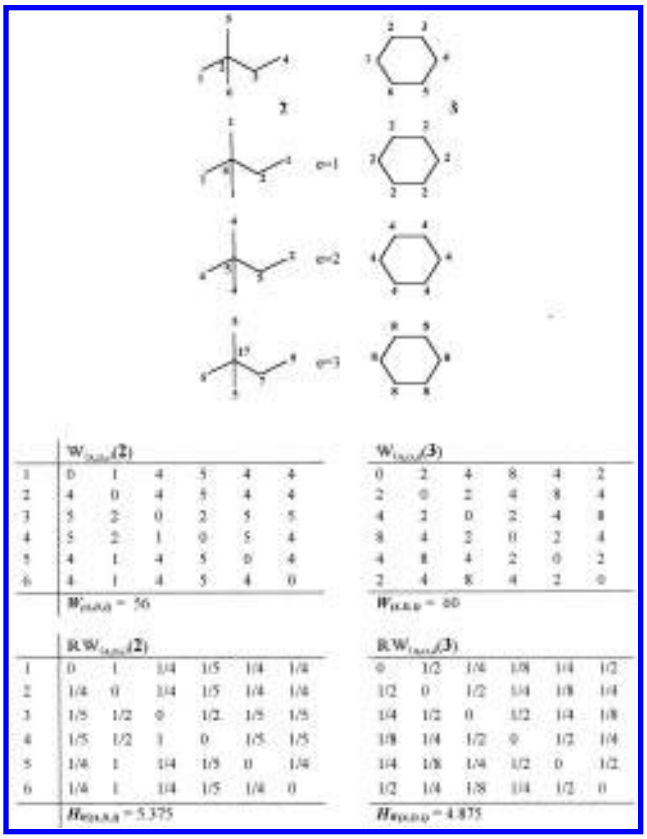


Figure 2. Graphs 2 and 3 (and their weighted graphs $\{^eW_{A,i}\}$; e = 1−3) and their matrices $W_{(A,D,1)}$ and $RW_{(A,D,1)}$.

definition (basically a relation of the type 4) for paths of any length in graph. It results in a *hyper-Wiener* number, $\boldsymbol{W_p}$ (as half sum of entries in the W_p matrix—see eq 14).

Table 1. Boiling Points, Wiener- and Harary-Type Indices for Some Cycloalkanes

no.	graph[a]	**BP**[b]	D_e	D_p	SZ_e	SZ_p	CJ_p	H_{De}	H_{Dp}	H_{SZe}	H_{SZp}	H_{CJp}
1	13MC5	94.5	41	68	51	147	119	13.083	10.767	1.000	3.278	5.000
2	MC6	100.9	42	71	78	182	142	12.917	10.600	0.667	3.083	4.167
3	C7	117	42	70	63	189	154	12.833	10.500	0.778	2.333	3.306
4	PC5	131	67	135	78	296	215	15.567	12.367	0.943	2.965	4.365
5	EC6	131.8	64	122	109	308	226	15.783	12.533	0.626	3.046	4.485
6	MC7	134	61	109	88	306	225	16.000	12.700	0.754	2.810	4.615
7	112MC5	114	56	92	67	218	150	16.667	13.333	1.004	5.101	9.279
8	113MC5	105	58	100	71	240	170	16.500	13.200	0.970	4.612	7.745
9	123MC5	115	58	99	70	230	164	16.417	13.100	0.956	3.862	8.218
10	1M2EC5	124	61	110	72	247	178	16.083	12.800	0.944	3.547	6.494
11	1M3EC5	121	63	119	76	270	199	15.950	12.700	0.911	3.169	5.502
12	IPC5	126.4	62	114	73	278	186	16.000	12.733	1.002	4.041	5.941
13	11MC6	120	59	103	104	284	197	16.333	13.033	0.686	4.691	6.727
14	12MC6	124	60	106	106	*296*	202	16.167	12.867	0.677	3.611	6.455
15	13MC6	120	61	110	108	*296*	211	16.083	12.800	0.669	3.544	5.780
16	14MC6	120	62	115	110	310	220	16.033	12.767	0.661	3.372	5.605
17	C8	146	64	120	128	364	288	15.667	12.400	0.500	2.333	3.278
18	1123MC5	132.7	78	137	93	358	222	20.167	15.700	0.938	5.158	11.925
19	113MC6	136.6	82	152	140	*447*	285	19.750	15.333	0.686	5.036	8.744
20	124MC6	136	*84*	160	*144*	474	296	19.533	15.133	*0.675*	3.803	8.392
21	135MC6	138.5	*84*	159	*144*	*447*	291	19.500	15.100	*0.675*	3.958	8.375
22	1M2EC6	151	86	167	*142*	460	300	19.283	14.900	0.645	3.638	7.178
23	1M3EC6	149	*88*	*176*	146	481	322	19.150	14.800	0.633	3.432	6.292
24	PC6	154	94	203	148	508	352	18.683	14.414	0.585	3.027	4.723
25	IPC6	146	*88*	*176*	*142*	487	313	19.150	14.800	0.639	4.100	6.583
26	EC7	163.5	*88*	175	121	484	337	19.067	14.700	0.708	2.849	5.028
27	C9	170	90	180	*144*	576	450	18.750	14.400	0.563	2.250	3.125
28	13EC6	170.5	121	263	192	735	467	22.383	16.848	0.603	3.325	6.932
29	PC7	183.5	124	277	163	757	503	22.133	16.629	0.666	2.858	5.194
30	C10	201	125	275	250	945	705	21.833	16.333	0.400	2.250	3.317

[a] M = methyl; E = ethyl; P = propyl; IP = isopropyl. [b] From ref 51.

Another way to evaluate this hyper-number is from the combinatorial matrix,[20] $\mathbf{D_p}$ (i.e., distance-path matrix—see eq 15) whose entries count all the "internal" paths included in a path **(i,j)**, (eq 16)

$$\boldsymbol{W_p} = \mathbf{(1/2)}\sum_{\mathbf{i}}\sum_{\mathbf{j}} [\mathrm{W_p}]_{\mathbf{ij}} \tag{14}$$

$$\boldsymbol{D_p} = \mathbf{(1/2)}\sum_{\mathbf{i}}\sum_{\mathbf{j}} [\mathrm{D_p}]_{\mathbf{ij}} \tag{15}$$

$$[\mathrm{D_P}]_{\mathbf{ij}} = \binom{[\mathrm{D_e}]_{\mathbf{ij}} + \mathbf{1}}{\mathbf{2}} \tag{16}$$

The hyper-number, $\boldsymbol{W_p}$, is calculable only in acyclic structures, whereas the $\boldsymbol{D_p}$ number is calculable in any graph. We stress that both hyper-numbers, when calculable, give one and the same hyper-Wiener value. Hyper-numbers on the Szeged and Cluj matrices were also calculated, as shown in Figure 1 and Table 1.[16,18]

A *hyper-Harary number* can be constructed by considering the reciprocal of the property collected by a path-defined matrix, $\mathrm{M_p}$. Thus, it can be defined as

$$\boldsymbol{H_{Mp}} = \mathbf{(1/2)}\sum_{\mathbf{i}}\sum_{\mathbf{j}} [\mathrm{RM_p}]_{\mathbf{ij}} \tag{17}$$

It is well-known the equality of the sum of the paths external and internal with respect to all paths in a tree graph; it leads to the equality of the Wiener indices (i.e., $\boldsymbol{W_e} = \boldsymbol{D_e}$ and $\boldsymbol{W_p} = \boldsymbol{D_p}$). The reciprocal properties, and the corresponding Harary numbers, do not obey such a relation (i.e., $\boldsymbol{H_{We}} \neq \boldsymbol{H_{De}}$ and $\boldsymbol{H_{Wp}} \neq \boldsymbol{H_{Dp}}$—see also Table 2). However, the Harary indices are intercorrelated (within the set of octanes), as can be seen from the subsequent matrix: the edge-defined Harary indices, $\boldsymbol{H_{De}}$ and $\boldsymbol{H_{We}}$, are highly correlated (i.e., over 0.99) with the corresponding path-defined ones (i.e., hyper-Harary indices) and the two hyper-Harary indices are highly correlated with each other.

Chart 1. Intercorrelating Matrix of Harary-Type Indices in Octanes

	H_{De}	H_{We}	H_{Dp}	H_{Wp}
H_{De}	**1**	**0.9865**	**0.9989**	**0.9898**
H_{We}		**1**	**0.9847**	**0.9968**
H_{Dp}			**1**	**0.9905**
H_{Wp}				**1**

Matrices of the reciprocal Szeged and Cluj descriptors offer the hyper-indices $\boldsymbol{H_{SZp}}$ and $\boldsymbol{H_{CJp}}$. In trees, $\boldsymbol{H_{CJp}} = \boldsymbol{H_{Wp}}$. The number $\boldsymbol{H_{SZp}}$ shows an interesting pairwise degeneracy in simple cycles, $\mathbf{C_{N,\ odd}}$, $\mathbf{C_{N+1}}$ (see Table 2, entry 18).

$\boldsymbol{H_{W(A,D,1)}}$ is a hyper-number by virtue of the construction of the basic matrix, $\mathrm{W_{(A,D,1)}}$. The index is calculated from the $\mathrm{RW_{(A,D,1)}}$ matrix, (which is identical to the "restricted random walk" matrix of Randić[23]) by applying the summative orthogonal operator (i.e., $\sum_{(\mathbf{i,j})}([\mathrm{M_u}]_{\mathbf{ij}} + [\mathrm{M_u}]_{\mathbf{ji}})$). Note that a hyper-Harary analogue was proposed in ref 24.

Values of hyper-Harary numbers are included in Tables 1 and 6 (see below).

ANALYTICAL RELATIONS FOR THE WIENER- AND HARARY-TYPE INDICES IN PATHS, CYCLES, AND STARS

The analysis of matrices of the basic and reciprocal properties (supplied by the computer programs TOP and CLUJ, written in Turbo Pascal and MAPLE V, respectively) enabled the writing of the sums leading to the herein discussed indices (Table 2). Most of these sums could be transformed into the corresponding analytical relations, by means of the MAPLE V (release 2) algebraic program.

Table 2. Analytical Relations for Wiener- and Harary-Type Indices in Paths, Cycles, and Stars

Index	Sums	Final Relations	Examples
Paths			
1 D_e	$\sum_{i=1}^{N-1}(N-i)i$	$\frac{1}{6}N(N-1)(N+1)$	N=11 220
2 H_{De}	$\sum_{i=1}^{N-1}(N-i)i^{-1}$	$-N+N\Psi(N)+1+N\gamma$	N=11 22.219
3 D_p	$\sum_{i=1}^{N-1}(N-i)\binom{i+1}{2}$	$\frac{1}{24}N(N-1)(N+2)(N+1)$	N=11 715
4 H_{Dp}	$\sum_{i=1}^{N-1}(N-i)\binom{i+1}{2}^{-1}$	$-2\Psi(N+1)+2N-2\gamma$	N=11 15.96
5 W_e; SZ_e; CJ_e	$\sum_{i=1}^{N-1}(N-i)i$	$\frac{1}{6}N(N-1)(N+1)$	N=11 220
6 H_{We}; H_{SZe}; H_{CJe}	$\sum_{i=1}^{N-1}(N-i)^{-1}i^{-1}$		N=11 0.533
7 W_p; CJ_p	$\sum_{i=1}^{N-1}\sum_{j=1}^{N-1}ij$	$\frac{1}{24}N(N-1)(N+2)(N+1)$	N=11 715
8 H_{Wp}; H_{CJp}	$\sum_{i=1}^{N-1}\sum_{j=1}^{N-1}i^{-1}j^{-1}$		N=11 7.562
9 SZ_p	$\sum_{i=1}^{N-1}(N-i)i+\sum_{i=1}^{\binom{N-z}{2}+z-1}i(N-i-1)i+\sum_{i=1}^{N-2}(N-i-1)(N-i-1)i+\sum_{i=1}^{\binom{N-z}{2}+z-1}i(N-i-1)(i+1)+\sum_{i=1}^{N-2}(N-i-2)(N-i-1)(i+1)$	$\frac{1}{48}(5N^4-10N^3+16N^2-8N-6Nz+3z)$	N=11 1285; N=12 1846
10 H_{SZp}	$\sum_{i=1}^{N-1}(N-i)^{-1}i^{-1}+\sum_{i=1}^{\binom{N-z}{2}+z-1}i(N-i-1)^{-1}i^{-1}+\sum_{i=1}^{N-2}(N-i-1)(N-i-1)^{-1}i^{-1}+\sum_{i=1}^{\binom{N-z}{2}-1}i(N-i-1)^{-1}(i+1)^{-1}+\sum_{i=1}^{N-2}(N-i-2)(N-i-1)^{-1}(i+1)^{-1}$		N=11 2.583; N=12 2.598
Cycles			
11 D_e	$N\sum_{i=1}^{\binom{N-z}{2}}i-(1-z)\binom{N-z}{2}\binom{N-z}{2}$	$\frac{1}{8}N(N^2-z)$	N=11 165; N=12 216
12 H_{De}	$N\sum_{i=1}^{\binom{N-z}{2}}i^{-1}-(1-z)\binom{N-z}{2}\binom{N-z}{2}^{-1}$	$N\left(\Psi\left(\frac{1}{2}N-\frac{1}{2}z+1\right)+\gamma\right)-1+z$	N=11 25.117; N=12 28.4
13 D_p	$N\sum_{i=1}^{\binom{N-z}{2}}\binom{i+1}{2}-(1-z)\binom{N-z}{2}\binom{N-z}{2}+1$	$\frac{1}{48}(N-z)(N-z+1)(N-z+2)(N+3z)$	N=11 385; N=12 546
14 H_{Dp}	$N\sum_{i=1}^{\binom{N-z}{2}}\binom{i+1}{2}^{-1}-(1-z)\binom{N-z}{2}\binom{N-z}{2}+1^{-1}$	$2\frac{(N^2-Nz+2z-2)}{(N-z+2)}$	N=11 18.333; N=12 20.286
15 SZ_e	$N\left(\frac{N-z}{2}\right)^2$	$\frac{1}{4}N(N-z)^2$	N=11 275; N=12 432
16 H_{SZe}	$N\left(\frac{N-z}{2}\right)^2$	$4\frac{N}{(N-z)^2}$	N=11 0.44; N=12 0.333
17 SZ_p	$N\frac{N-1}{2}\left(\frac{N-z}{2}\right)^2-2(1-z)\left(\frac{N-z}{2}\right)\left[\left(\frac{N-z}{2}\right)^2-\left(\frac{N-z}{2}-1\right)^2\right]$	$\frac{1}{8}N(N-1)^{(2z+1)}(N^2-2N+4)^{(1-z)}$	N=11 1375; N=12 2046
18 H_{SZp}	$N\frac{N-1}{2}\left(\frac{N-z}{2}\right)^{-2}-2(1-z)\left(\frac{N-z}{2}\right)\left[\left(\frac{N-z}{2}\right)^{-2}-\left(\frac{N-z}{2}-1\right)^{-2}\right]$	$\frac{N-1+z}{(N-2+z)/2}$	N=11 2.2; N=12 2.2
19 CJ_p	$(1-z)N\left(\frac{N-z}{2}\right)^2+2N\sum_{i=1-z}^{\left(\frac{N-z}{4}\right)\left(1-\frac{y-z}{4}\right)}\left(\frac{N-z}{2}-i\right)^2+(1-y)\frac{N}{2}\left(\frac{N-z}{2}-\left(\frac{N-z}{4}-\frac{y-z}{4}\right)\right)^2$	$\frac{1}{96}N(72z^2N-9y^2N-16z^3-3y^2-12yz^2+12yzN+12y^2z-3N^2-2y^3+7N^3+8N+8y-108zN+12z^2+18yN-12yz+16z)$	N=9; 10; 11; 12; CJ_p = 450; 705; 1001; 1470
20 H_{CJp}	$(1-z)N\left(\frac{N-z}{2}\right)^{-2}+2N\sum_{i=1-z}^{\left(\frac{N-z}{4}\right)\left(1-\frac{y-z}{4}\right)}\left(\frac{N-z}{2}-i\right)^{-2}+(1-y)\frac{N}{2}\left(\frac{N-z}{2}-\left(\frac{N-z}{4}-\frac{y-z}{4}\right)\right)^{-2}$		
20 H_{CJp}	$\frac{4(1-z)N}{(N-z)^2}+2N\left(\Psi\left(1,1-\frac{z}{2}-\frac{N}{2}\right)-\Psi\left(1,\frac{y}{4}-\frac{N}{4}\right)\right)+\frac{8(1-y)N}{(N-2z+y)^2}$	N = 9; 10; 11; 12; H_{CJp} = 3.125; 3.317; 3.477; 3.460	
21 $W_{(A,D,I)}$	$\frac{1}{2}N\sum_{i=1}^{\binom{N-z}{2}-1}(2^i+2^{-i})+\frac{1}{2}\frac{N}{2-z}\left(2^{\frac{N-z}{2}}+2^{\frac{N-z}{2}}\right)$	$N\left(\frac{3*2^{\binom{N-z}{2}}-2^{\binom{N-z}{2}}z-4+2z}{2-z}\right)$	N=11 682; N=12 1128
22 $H_{W(A,D,I)}$	$\frac{1}{2}N\sum_{i=1}^{\binom{N-z}{2}-1}(2^{-i}+2^{-i})+\frac{1}{2}\frac{N}{2-z}\left(2^{\frac{N-z}{2}}+2^{\frac{N-z}{2}}\right)$	$N\left(\frac{-3*2^{\binom{-N+z}{2}}-2*2^{\binom{-N+z}{2}}z+2-z}{2-z}\right)$	N=11 10.656; N=12 11.719
Stars			
23 D_a	$N-1+\sum_{i=1}^{N-2}i*2$	$(N-1)^2$	N=11 100
24 H_{De}	$N-1+\sum_{i=1}^{N-2}i*2^{-1}$	$\frac{1}{4}(N+2)(N-1)$	N=11 32.5
25 D_p	$N-1+\sum_{i=1}^{N-2}i*3$	$\frac{1}{2}(N-1)(3N-4)$	N=11 145
26 H_{Dp}	$N-1+\sum_{i=1}^{N-2}i*3^{-1}$	$\frac{1}{6}(N+4)(N-1)$	N=11 25
27 W_e; Sz_e; CJ_e	$(N-1)(1*(N-1))$	$(N-1)^2$	N=11 100
28 H_{We}; H_{SZe}; H_{CJe}	$(N-1)(1*(N-1)^{-1})$	1	N=11 1
29 W_p; Sz_p; CJ_p	$(N-1)(1*(N-1))+\sum_{i=1}^{N-2}i*1*1$	$\frac{1}{2}(N-1)(3N-4)$	N=11 145
30 H_{Wp}; H_{SZp}; H_{CJp}	$(N-1)(1*(N-1)^{-1})+\sum_{i=1}^{N-2}i*1*1$	$\frac{1}{2}(N^2-3N+4)$	N=11 46
31 $W_{(A,D,I)}$	$\frac{1}{2}(N-1)(1+(N-1))+\sum_{i=1}^{N-2}i(N-1)$	$\frac{1}{2}(N-1)(N^2-2N+2)$	N=11 505
32 $H_{W(A,D,I)}$	$\frac{1}{2}(N-1)(1+(N-1)^{-1})+\sum_{i=1}^{N-2}i(N-1)^{-1}$	$N-1$	N=11 10

[a] $y = N \bmod 4$; $z = N \bmod 2$; $\gamma(x) = \text{int}(\exp(-t)*t\wedge(x-1), t = 0, \text{infinity}$; $\psi(x) = \text{diff}(\ln(\gamma(x),x)$; $\psi(n,x) = \text{diff}(\psi(x), x\$n)$; $\psi(0,x) = \psi(x)$.

However, formulas for the H_{We}, H_{Wp}, and H_{SZp}, in path graphs (entries 6, 8, and 10), could not be derived. There are some relations for the Harary-type indices (entries 2, 4, 12, and 20,) which involve the well-known gamma, digamma and polygamma functions (given in MAPLE language, at the end of Table 2). All the listed relations were verified, as numerical values (given as examples in Table 2), by means of both MAPLE and the original programs.

Table 3. Interrelating Formulas

	Graph	Relation	Graph	Relation
1	Paths	$D_p = \frac{1}{4}(N+2)D_e$	9 Stars	$H_{Wp} = H_{We} + \binom{N-1}{2}$
2		$D_p = D_e + \binom{N+1}{4}$	10	$H_{De} = \frac{1}{4}\frac{N+2}{N-1}D_e$
3	Cycles	$SZ_e = 2\frac{(N-z)^2}{N^2-z}D_e$	11	$H_{Dp} = \frac{1}{3}\frac{N+4}{3N-4}D_p$
4		$H_{SZp} = \frac{1}{2}N^{(1/2)}(N-1)(N-2)^{(x-1)}H_{Sze}$	12	$H_{We} = W_e - N(N-2)$
5	Stars	$D_p = \frac{1}{2}\frac{3N-4}{N-1}D_e$	13	$H_{Wp} = \frac{N^2}{2} - \frac{W_p}{N-1}$
6		$H_{Dp} = \frac{2}{3}\frac{N+4}{N+2}H_{De}$	14	$H_{W(A,D,1)} = W_{(A,D,1)} + \frac{2}{N^2-2N+2}$
7		$H_{We} = N - W_e^{1/2}$	15	$H_{W(A,D,1)} = \frac{6H_{Dp}}{N+4}$
8		$H_{W(A,D,1)} = N - H_{We} = W_e^{1/2}$	16	$H_{W(A,D,1)} = \frac{2W_p}{3N-4}$

Several relations which interrelate the herein discussed indices have been derived, and are presented in Table 3.

An interesting recursive relation, obeyed in path graphs by the W_p index

$$W_p(N) = W_e(N) + W_p(N-1) \tag{18}$$

and resulting from the combinatorial relation

$$\binom{N+2}{4} = \binom{N+1}{3} + \binom{N+1}{4} \tag{19}$$

is maintained in the case of the corresponding Harary index

$$H_{Wp}(N) = H_{We}(N) + H_{Wp}(N-1) \tag{20}$$

Expansion of relation 20 leads to a composition relation for this hyper-Harary index

$$H_{Wp}(N) = H_{We}(1) + H_{We}(2) + ... + H_{We}(N) \tag{21}$$

which is equivalent to that found by Lukovits[25] for the basic property index, W_p (see also ref 20). Despite the equality $D_p = W_p$ (compare eqs 18 and 19 and entry 2 in Table 3), a relation equivalent to (21) for the H_{Dp} index was not found. Some relations for the basic property indices, included in Table 2, can be found in refs 10, 20, and 25.

CORRELATING AND DISCRIMINATING TESTS

Correlating ability is one of the most important requirement of a molecular descriptor.[26] It has to be associated with the direct structural interpretation for making a given descriptor useful in the investigation of structure−property relation.

While the basic property indices, shown in Table 1, correlate (in single variable regression) at most 0.958 (CJ_p index) with the boiling point, **BP**, of a selected set of cycloalkanes, the reciprocal property indices do not overpass 0.821 (see Table 4). It is obvious that neither the basic indices nor the reciprocal property ones are good enough for predicting purposes.

Attempts to find a satisfactory correlation, in two variable regression, by using the basic indices, failed (see Table 4, entries 11−13). Significant improvement was recorded when two Harary-type indices were associated (entries 14−16). The best correlation ($r = 0.978$; $s = 5.297$; $F = 291.951$) was obtained with H_{De} and H_{CJp} (entry 16). The *cross validation* test (let 1/3 out) on this equation offered a **r** value of 0.97, indicating a good prediction ability.

Table 4. Statistics of Regressions ($Y = a + \sum_i b_i X_i$; **Y** = **BP**) of the Parameters Listed in Table 1

	X	r	s	F	a	b
1	D_e	0.931	9.034	182.024		
2	D_p	0.935	8.810	192.818		
3	SZ_e	0.886	11.495	101.708		
4	SZ_p	0.954	7.391	285.765		
5	CJ_p	0.958	7.100	312.027		
6	H_{De}	0.821	14.118	57.996		
7	H_{Dp}	0.788	15.232	45.879		
8	H_{SZe}	0.667	18.435	22.434		
9	H_{SZp}	0.412	22.539	5.739		
10	H_{CJp}	0.238	24.030	1.684		
11	D_e	0.935	8.955	93.366	74.684	0.210
	D_p					0.322
12	D_e	0.964	6.660	179.691	76.750	0.327
	CJ_p					0.130
13	SZ_e	0.957	7.300	147.463	90.537	−0.132
	SZ_p					0.156
14	H_{De}	0.970	6.094	217.277	266.220	87.876
	H_{Dp}					−121.645
15	H_{De}	0.966	6.558	185.742	42.994	8.349
	H_{SZp}					−15.069
16	H_{De}	0.978	5.297	291.951	10.429	9.517
	H_{CJp}					−6.663

The enthalpy of cycloalkanes C_6−C_{17} is well correlated with the following Harary indices: H_{De}, $r = 0.983$; $s = 17.209$; $F = 278.843$; H_{De} and H_{Dp}, $r = 0.991$; $s = 13.210$; $F = 240.584$; H_{De} and H_{SZp}, $r = 0.993$; $s = 11.178$; $F = 337.818$.

The index H_{We} shows an excellent correlation with the octane number, **ON**, both in linear ($r = 0.971$; $s = 6.099$; $F = 231.737$) and parabolic ($r = 0.991$; $s = 3.541$; $F = 357.924$) regression. In parabolic regression, the hyper-Harary index, H_{Wp}, shows the best correlation with the octane number ($r = 0.9922$; $s = 3.313$; $F = 409.967$) among all the tested indices.

van der Waals area of octanes, in single variable regression, is best (but not satisfactory) described by the Bertz index,[27] B_2 (i.e., the number of edges in the second line derivative): $r = 0.921$; $s = 1.346$; $F = 88.755$. A close correlation is given by H_{Dp}: $r = 0.915$; $s = 1.386$; $F = 82.770$.

In two variable regression, B_2 associated with the classical topological indices, does not overpass $r = 0.93$. It is succeeded by two Harary-type indices, H_{SZp} and $H_{W(AD1)}$ (in single variable regression: $r = 0.889$; $s = 1.576$, and $r = 0.804$; $s = 2.048$, respectively): $r = 0.9727$; $s = 0.825$; $F = 131.856$ (note the significant dropping of the standard error of estimate, **s**).

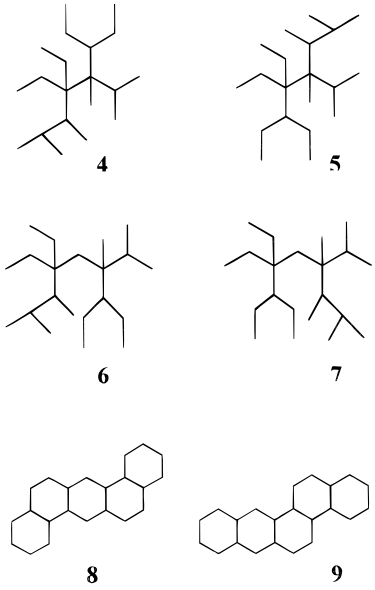
H_{We} and H_{SZe} show the same degeneracy in octanes as the Wiener index, but the hyper-Harary indices possess a better ability in discriminating isomers, resulting from a study performed on the set of all cycloalkanes with ten vertices/atoms and having 3−10 membered cycles (439 structures). We have evaluated the *sensitivity* number, **S**, according to

$$S = n_d/n \tag{22}$$

where n_d is the number of distinct values of an index and **n** is the whole number of structures investigated.[28,29] Table 5 collects the sensitivity numbers for all the basic and the corresponding Harary indices herein discussed, both on subsets of a given membered cycle and on the whole set of

Table 5. Discriminating Sensitivity Number for Wiener and Harary Indices

	index	Cy3 n = 168	Cy4 n = 140	Cy5 n = 70	Cy6 n = 40	Cy7 n = 13	Cy8 n = 6	Cy3-10 n = 439
1	D_e	0.244	0.286	0.400	0.550	0.692	1	0.116
2	H_{De}	0.619	0.629	0.786	0.700	0.923	1	0.355
3	D_p	0.637	0.579	0.786	0.725	0.923	1	0.339
4	H_{Dp}	0.655	0.671	0.729	0.800	0.923	1	0.376
5	SZ_e	0.256	0.321	0.400	0.525	0.846	1	0.223
6	H_{SZe}	0.804	0.764	0.929	0.825	0.846	1	0.788
7	SZ_p	0.685	0.779	0.629	0.725	0.923	0.833	0.483
8	H_{SZp}	0.994	1	1	1	1	1	0.995
9	CJ_p	0.667	0.757	0.771	0.975	0.923	1	0.476
10	H_{CJp}	1	1	1	1	1	1	1
11	$W_{(A,D,1)}$	0.893	0.836	0.929	0.950	0.923	1	0.733
12	$H_{W(A,D,1)}$)	0.994	0.993	1	1	1	1	0.995
13	J	0.994	0.971	1	0.950	1	1	0.984



2*DDS:

(**4; 5**): 38, 56, 82, 92, 72, 32, 8

(**6; 7**): 40, 58, 76, 78, 72, 56, 32, 8

(**8; 9**): 52, 76, 82, 68, 56, 44, 34, 24, 16, 8, 2

Figure 3. Pairs of graphs with pairwise identical Distance Degree Sequence, DDS, and degenerate topological indices (see Table 6).

Table 6. Topological Indices for the Graphs 4−9 in Figure 3

	graph					
I	4	5	6	7	8	9
W_e	686	686	840	840		
W_p	1797	1797	2445	2445		
D_e	686	686	840	840	971	971
D_p	1797	1797	2445	2445	3162	3162
SZ_e	686	686	840	840	2354	2354
SZ_p	9610	9610	13848	13848	19993	19908
CJ_e	686	686	840	840	2354	2354
CJ_p	1797	1797	2445	2445	13644	13558
$W_{(A,D,1)}$	6028	6028	12185	12185	77582	76273
H_{We}	0.7133	0.7133	0.6855	0.6855		
H_{Wp}	78.0175	78.0175	79.1364	79.1364		
H_{De}	68.6048	68.6048	71.5690	71.5690	81.7417	81.7417
H_{Dp}	43.0714	43.0714	44.3159	44.3159	53.0204	53.0204
H_{SZe}	0.7133	0.7133	0.6855	0.6855	0.3152	0.3131
H_{SZp}	8.9836	8.9836	8.5340	8.5340	3.6428	3.5975
H_{CJe}	0.7133	0.7133	0.6855	0.6855	0.3152	0.3131
H_{CJp}	78.0175	78.0175	79.1364	79.1364	4.9707	4.9366
$H_{W(A,D,1)}$	14.2001	14.2215	13.1552	13.1736	8.7162	9.1239

isomers. In comparison, another simple index is considered: the highly discriminating index of Balaban,[30] ***J***.

As it can be seen from Table 5, all the Harary indices have a more discriminating power than the corresponding basic indices.

There are, however, pairs of graphs with identical distance degree sequences, **DDS,** which induce degeneracy in most indices based on distances in a graph, even they are indices of reciprocal property. Graphs **4**−**7** in Figure 3 were so built up by Ivanciuc[31] to possess such a property: all indices listed in Table 6 show pairwise degenerate values, except $\boldsymbol{H_{W(A,D,1)}}$. Similarly, the cycle-containing pair[32] **8;9** shows degeneracy for the following indices: $\boldsymbol{D_e}$, $\boldsymbol{D_p}$, $\boldsymbol{SZ_e}$, $\boldsymbol{CJ_e}$, $\boldsymbol{H_{De}}$, and $\boldsymbol{H_{Dp}}$.This pair is well discriminated by the hyper-indices $\boldsymbol{SZ_p}$, $\boldsymbol{CJ_p}$, and $\boldsymbol{W_{(A,D,1)}}$ and most of the Harary indices.

DISCUSSION

As the number of topological indices (i.e., single number molecular descriptors) continuously increases, two divergent opinions are manifested: (i) to stop the hazardous proliferation of these indices[26,33−35] and (ii) to use a wide poll of indices in multivariate regression analysis, with the aim of finding the best description of a given property.[36,37]

The first opinion emerged, on the one hand, from the lack (or no general acceptance) of a systematic search for novel molecular descriptors and, on the other hand, from the older idea that a good index has to be a simple (i.e., easily calculable) index. In this respect, Randić has published[26] a list of desirable attributes for topological indices. Among these requirements, the first three (1. "Direct structural interpretation"; 2. "good correlation with at least one property"; 3. "good discrimination of isomers") are by far the most important.

The second opinion has resulted from a more pragmatic reason: a molecular property is more often a function of two or more variables. A best correlation once found is not a strong reason for breaking the search for an even better correlation. Consequently, the "race" for better and better indices continues. It is not a surprise that the program CODESSA of Lobanov[37] is able to supply 600 molecular descriptors.

In our opinion, a new molecular descriptor is always justified if the first three attributes stated by Randić (see above) are fulfilled. If it is built up on chemical graphs, it will necessarily be related to the chemical structure (see the first requirement), although this relation could be more or less transparent.[26]

The correlating ability is a desiderate which, in single variable, is rarely reached. Studies of Randić on octanes[38] showed that properties such as boiling points, critical pressure, etc. can be projected on a p_2/p_3 grid (p_2 and p_3 being the number of paths of length 2 and 3, respectively). A good statistical quality of a regression equation requires, however, more than two independent variables. If its explicative role about a given property is rather easily fulfilled (e.g., a causal relation structure−property is conceivable at a value of correlation coefficient, **r**, greater than 0.80), the predictive role of such an equation will be attained only by the insight into the "dimensionality" of that property. The best predictive equation found by Smeeks and Jurs[36] by investigating a large set of aliphatic alcohols contains seven structural descriptors, and this is not a singular example.[39]

The third requirement is, mainly, a function of the graph invariants taken into account. Compare, in this respect, the Randić's index, χ (ref 40), and the Balaban's index, ***J*** (ref 30): both use the same mathematical operation (reciprocal square root), but the first is built up on vertex degrees, while the second on distance weighted vertex degrees (i.e., sum of distances from a vertex **i** to all other vertices in a graph). While χ is rather degenerate within the alkane isomers (first degenerate pairs occurring in octanes), ***J*** is a highly discriminating index (first degenerate values being recorded in dodecanes). The mathematical operation play a secondary role: compare the Zagreb group index,[41] M_2 (which is the sum, over all edges **(i,j)** in graph, of the vertex degree products, **deg(i)*deg(j)**), with χ index (which is the reciprocal square root of the same product), the last one being less degenerate. An additional proof in this respect is provided by the data included in Table 6: pairs of graphs **4;5** and **6;7** having pairwise identical **DDS** show degenerate values of the indices (except $H_{W(A,D,1)}$) calculated from both basic and reciprocal properties involving distances in a graph.

The proposal of the novel Harary-type indices herein presented is justified as follows: (i) indices are constructed on chemical graphs (i.e., alkanes) on a matrix ground. Further development of the basic property indices, CJ_p and SZ_p, which takes into account chemical fragments,[42] will allow the calculation of Harary indices on chemical structures including multiple bonds and heteroatoms; (ii) they are suitable for correlating tests, particularly in multivariate regression; (iii) reciprocal numbers summed as Harary indices relieve (or lower) the degeneracy occurring in the case of the basic property indices (see Table 1−the italicized values−and Table 5). Hyper-Harary indices show a more discriminating ability than the edge-defined indices (compare H_{SZe} with H_{SZp} and H_{CJp}−Tables 1 and 5). Among the 13 indices tested on the set of 439 cycloalkanes with ten vertices, H_{CJp} was the only index with the sensitivity 1. It is followed by H_{SZp} and $H_{W(A,D,1)}$ (0.995) which are, at least within the considered set, more discriminating than the ***J*** index (0.984). Taking into account the following facts: (i) ***J*** shows the first degenerate values in dodecanes;[43] (ii) in a set of 5002 unbranched hexagonal structures tested by Konstantinova[44] it shows six pairs of degenerate values; and (iii) in the set of 439 cycloalkanes seven such pairs are encountered, one can appreciate that our set is more difficult to separate than the above mentioned sets. This result proves the good discriminating ability of the newly proposed Harary indices. We stress here that the Harary indices cannot be, however, compared with the ***ID*** (identification) super-indices,[45−49] or with the most powerful ***EAID*** number of Hu and Xu,[50] which discriminated among over 4 000 000 chemical structures. Cycloalkane isomers have been generated by the program FRAGGEN, written in Turbo Pascal.

Our indices are strongly based on graph theoretical invariants (in contrast with some indices−e.g., "the three-dimensional valence connectivity index" $\Omega(q)$, of Estrada[33]−which are hybrids of quantum-chemical and graph theoretical calculations) so that their structural interpretation is straightforward.

Investigation of the mathematical properties of Harary indices in three classes of graphs, paths, simple cycles, and stars, led to interesting results. More than half of the number of reciprocal property indices could be expressed by simple analytical relations, but in some cases (entries 2, 4, 12, and 20−Table 2) more complex functions were needed. However, in path graphs, such relations could not be found for three indices: H_{We}, H_{Wp}, and H_{SZp} (entries 6, 8, and 10).

Convergence behavior of some Harary indices is particularly nice. In cycles, the hyper-Cluj index,[18] CJ_p, is a function of **N mod 4** (Table 2, entry 19). The reciprocal property index, H_{CJp} (Table 2, entry 20), shows the limit **4**, when **N** tends toward infinity. Moreover, it shows a particular periodicity according to the four values of **N mod 4**. These facts explain the low correlation of this index, in single variable regression.

Another interesting trend is offered by $H_{W(AD1)}$. In cycles, this index can be written as the product **N*f(N,z)** (cf. Table 2, entry 22): since

$$\lim_{N\to\infty} \mathbf{f(N,z)} = 1$$

the values of this index reach **N**, rather quickly (in three decimals, starting with $\mathbf{N} = 34$).

In star graphs, H_{We} (and also H_{SZe} and H_{CJe}) is a constant (e.g., unity).

CONCLUSIONS

Harary indices, or indices of reciprocal properties, are distinct quantities, derived on a matrix ground, according to the graph theoretical concepts. Their construction was illustrated and examplified on a set of cycloalkanes. Analytical relations for their calculation in paths, cycles, and stars were derived. Correlating and discriminating ability of these indices was investigated, and limitations in this respect were admitted. The results presented in this paper indicate that the Harary indices are not simple artefacts but interesting tools in the investigation of molecular structures, which deserve further attention.

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