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DESIGN OF TOPOLOGICAL INDICES. Part 13[1]

STRUCTURAL DESCRIPTORS COMPUTED FROM THE SZEGED MOLECULAR MATRICES

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The Wiener index, equal to the sum of the molecular graph distances, is a widely used chemical descriptor for structure-property and structure-activity models. In recent years topological indices found new applications in drug design, database mining, similarity and diversity assessment. As a result of the considerable interest for topological indices, new molecular matrices were derived from graph distances: the reciprocal distance, resistance distance, distance-valency, Szeged, and Cluj matrices. We present several graph descriptors derived from the Szeged matrices: characteristic polynomials, matrix spectra, spectral moments. From the new descriptors, several can be used in structure-property and structure-activity models.

INTRODUCTION

Numerous structural descriptors are used to compute physical, chemical, or biological properties with quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) models. A significant fraction of the structural descriptors defined so far are derived from the molecular graph representation of chemical compounds. Molecular graphs are non-directed chemical graphs that represent, in different conventions, molecules. In molecular graphs vertices correspond to atoms and edges represent covalent bonds between atoms, while geometrical features of molecules, such as bond lengths or bond angles, are not considered. Numerous reviews[2–10] were published on the theory and applications of topological indices in QSPR and QSAR models. Using molecular graphs the chemical structure of a chemical compound can be expressed by means of various graph matrices, polynomials, spectra, spectral moments, sequences counting distances, paths, and walks, or topological indices. A topological index (TI) is a numerical descriptor of the molecular structure based on certain topological feature of the molecular graph. When compared with other classes of structural descriptors, such as geometric or quantum descriptors, topological indices have some important advantages because they can be easily computed from the molecular graph and they offer a simple way of measuring molecular branching, shape, and size. The Wiener index,[11] equal to the sum of the molecular graph distances, is a widely used chemical descriptor for structure-property and structure-activity models. The original formula for the Wiener index W can be applied only for alkanes; Hosoya proposed a formula based on the distance matrix for computing the Wiener index for cyclic molecular graphs.[12] In recent years topological indices based on graph distances found new applications in drug design, database mining, similarity and diversity assessment. As a result of the considerable interest for structural descriptors, new topological indices were derived from graph distances: the reciprocal distance matrix **RD**,[13–18] the Szeged index Sz,[19–27] and Szeged matrices.[28–32] In this paper we present several graph descriptors derived from the Szeged matrices: characteristic polynomials, matrix spectra, spectral moments. From the new descriptors, several can be used in structure-property and structure-activity models.

THE SZEGED INDEX AND THE SZEGED MATRICES

The original definition of the Wiener index W was formulated only for alkanes.[11] Consider an acyclic graph $G = G(V,E)$ and denote with N_i and N_j the number of vertices situated on both sides of the edge e_{ij}; vertex v_i is counted in N_i while vertex v_j is counted in N_j. For acyclic graphs the Wiener index $W = W(G)$ of a graph G is defined with the formula:

$$W(G) = \sum_{e_{ij} \in E(G)} N_i N_j \tag{1}$$

where the summation goes over all edges from the edge set $E(G)$, $e_{ij} \in E(G)$. Hosoya proposed an extension of the Wiener index for cyclic graphs:[12]

$$W(G) = \frac{1}{2} \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} [\mathbf{D}]_{ij}. \tag{2}$$

Gutman introduced another formula that can be used to compute the Wiener index for cyclic graphs. With a formula related to that used in equation (1) for the index W he introduced a new index, the Szeged index Sz.[19-22] The interest in the new index was high, and in a short time a remarkable research effort was made by mathematicians and chemists in order to elaborate the theory and applications of Sz.[23-27] The Szeged index is defined in the following way. Let e_{ij} be an edge of the molecular graph G, connecting the vertices v_i and v_j from G, $v_i, v_j \in V(G)$. Let n_i be the number of vertices v_k of the molecular graph G, having the property $d_{ki} < d_{kj}$ and let n_j be the number of vertices v_k of the molecular graph G, having the property $d_{kj} < d_{ki}$. When a vertex v_k is situated at the same distance from vertices v_i and v_j, i.e. $d_{ki} = d_{kj}$, the vertex is not counted neither in n_i nor in n_j. For the two vertices that form the edge e_{ij}, n_i gives the number of vertices closer to vertex v_i and n_j gives the number of vertices closer to vertex v_j. A formal definition of n_i and n_j is offered below:

$$n_i = \{v_k : v_i, v_j, v_k \in V(G), e_{ij} \in E(G), d_{ki} < d_{kj}\} \tag{3}$$

$$n_j = \{v_k : v_i, v_j, v_k \in V(G), e_{ij} \in E(G), d_{kj} < d_{ki}\}. \tag{4}$$

The Szeged index of the molecular graph G is:

$$Sz(G) = \sum_{e_{ij} \in E(G)} n_i n_j \tag{5}$$

where the summation goes over all edges e_{ij} from the edge set $E(G)$, $e_{ij} \in E(G)$. In acyclic graphs $N_i = n_i$ and $N_j = n_j$ and the Wiener and Szeged indices coincide.

Diudea proposed an extension of the equations (3) and (4) for any pair of vertices $v_i, v_j \in V(G)$.[28-32] In a graph G with N vertices labeled from 1 to N, n_{ij} represents the number of vertices v_k of the molecular graph G having the property $d_{ki} < d_{kj}$:

$$n_{ij} = \{v_k : v_i, v_j, v_k \in V(G), d_{ki} < d_{kj}\}. \tag{6}$$

This quantity is the element of the nonsymmetric Szeged matrix $\mathbf{Sz_u} = \mathbf{Sz_u}(G)$, a square $N \times N$ nonsymmetric matrix:

$$[\mathbf{Sz_u}]_{ij} = \begin{cases} n_{ij} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}. \tag{7}$$

The square $N \times N$ dense symmetric Szeged matrix $\mathbf{Sz_p} = \mathbf{Sz_p}(G)$ is obtained from $\mathbf{Sz_u}$ through a symmetrization operation:

$$[\mathbf{Sz_p}]_{ij} = \begin{cases} n_{ij} n_{ji} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}. \tag{8}$$

With a similar symmetrization operation one obtains from $\mathbf{Sz}_u$ the square $N\times N$ sparse symmetric Szeged matrix $\mathbf{Sz}_e = \mathbf{Sz}_e(G)$:

$$[\mathbf{Sz}_e]_{ij} = \begin{cases} n_{ij}n_{ji} & \text{if } i \neq j \text{ and } e_{ij} \in E(G) \\ 0 & \text{if } i = j \text{ or } e_{ij} \notin E(G) \end{cases} \tag{9}$$

where $E(G)$ represents the set of edges of G. An alternative definition of the $\mathbf{Sz}_e$ matrix is:

$$[\mathbf{Sz}_e]_{ij} = [\mathbf{A}]_{ij}n_{ij}n_{ji} = [\mathbf{A}]_{ij}[\mathbf{Sz}_p]_{ij} \tag{10}$$

where $[\mathbf{A}]_{ij}$ is the element of the adjacency matrix $\mathbf{A} = \mathbf{A}(G)$. The $\mathbf{Sz}_e$ and $\mathbf{Sz}_p$ matrices are used to define the Szeged, Sz, and the hyper-Szeged, Sz_p, indices of graph G:[28-32]

$$Sz = \sum_{i=1}^{N}\sum_{j=i}^{N}[\mathbf{Sz}_e]_{ij} \tag{11}$$

$$Sz_p = \sum_{i=1}^{N}\sum_{j=i}^{N}[\mathbf{Sz}_p]_{ij}. \tag{12}$$

The reciprocal Szeged matrix, $\mathbf{RSz}_p = \mathbf{RSz}_p(G)$, is a square $N\times N$ symmetric matrix derived from the $\mathbf{Sz}_p$ matrix:[28,31]

$$[\mathbf{RSz}_p]_{ij} = \begin{cases} [\mathbf{Sz}_p]_{ij}^{-1} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}. \tag{13}$$

POLYNOMIALS AND SPECTRA DERIVED FROM THE SZEGED MATRICES

The characteristic polynomial $\mathbf{Ch(M)} = \mathbf{Ch(M},G,x)$ of the molecular matrix $\mathbf{M} = \mathbf{M}(G)$ is defined with the following equation:[33]

$$\mathbf{Ch(M},G,x) = \mathbf{det}(x\mathbf{I} - \mathbf{M}) = \sum_{n=0}^{N} c_n x^{N-n} \tag{14}$$

where $\mathbf{I}$ is the unit matrix of order N and c_n is the nth coefficient of the characteristic polynomial $\mathbf{Ch(M)}$. The molecular graph of a normal alkane with N vertices is the linear graph L_N. The characteristic polynomials of the $\mathbf{Sz}_e$ matrices, $\mathbf{Ch}(\mathbf{Sz}_e)$, for the linear graphs L_3–L_{10} are given below.

$\mathbf{Ch}(\mathbf{Sz}_e,L_3) = x^3 - 8x$

$\mathbf{Ch}(\mathbf{Sz}_e,L_4) = x^4 - 34x^2 + 81$

$\mathbf{Ch}(\mathbf{Sz}_e,L_5) = x^5 - 104x^3 + 1408x$

$\mathbf{Ch}(\mathbf{Sz}_e,L_6) = x^6 - 259x^4 + 11971x^2 - 50625$

$\mathbf{Ch}(\mathbf{Sz}_e,L_7) = x^7 - 560x^5 + 68032x^3 - 1410048x$

$\mathbf{Ch}(\mathbf{Sz}_e,L_8) = x^8 - 1092x^6 + 295590x^4 - 18752644x^2 + 121550625$

$\mathbf{Ch}(\mathbf{Sz}_e,L_9) = x^9 - 1968x^7 + 1057728x^5 - 162280448x^3 + 4743069696x$

$\mathbf{Ch}(\mathbf{Sz}_e,L_{10}) = x^{10} - 3333x^8 + 3265482x^6 - 1045341514x^4 + 87561880389x^2 - 797493650625$

The molecular graph of a cycloalkane with N vertices is the ring R_N. We present below the characteristic polynomials of the $\mathbf{Sz_e}$ matrices, $\mathbf{Ch(Sz_e)}$, for the rings R_3–R_{10}.

$$\mathbf{Ch(Sz_e},R_3) = x^3 - 3x - 2$$

$$\mathbf{Ch(Sz_e},R_4) = x^4 - 64x^2$$

$$\mathbf{Ch(Sz_e},R_5) = x^5 - 80x^3 + 1280x - 2048$$

$$\mathbf{Ch(Sz_e},R_6) = x^6 - 486x^4 + 59049x^2 - 2125764$$

$$\mathbf{Ch(Sz_e},R_7) = x^7 - 567x^5 + 91854x^3 - 3720087x - 9565938$$

$$\mathbf{Ch(Sz_e},R_8) = x^8 - 2048x^6 + 1310720x^4 - 268435456x^2$$

$$\mathbf{Ch(Sz_e},R_9) = x^9 - 2304x^7 + 1769472x^5 - 503316480x^3 + 38654705664x - 137438953472$$

$$\mathbf{Ch(Sz_e},R_{10}) = x^{10} - 6250x^8 + 13671875x^6 - 12207031250x^4 + 3814697265625x^2 -$$

$$- 381469726562500$$

The $\mathbf{Ch(Sz_e)}$ polynomial has integer coefficients, with large positive or negative values. The coefficients of this polynomial increase rapidly with the increase of the number of atoms in the molecular graph. Without a scaling down, such structural invariants, are of little use in QSPR and QSAR studies. The values of the $\mathbf{Ch(Sz_p)}$ polynomial of the linear molecular graphs L_3–L_{10} are presented here.

$$\mathbf{Ch(Sz_p},L_3) = x^3 - 9x - 8$$

$$\mathbf{Ch(Sz_p},L_4) = x^4 - 58x^2 - 192x - 135$$

$$\mathbf{Ch(Sz_p},L_5) = x^5 - 226x^3 - 1848x^2 - 4968x - 4320$$

$$\mathbf{Ch(Sz_p},L_6) = x^6 - 725x^4 - 11632x^3 - 69996x^2 - 175504x - 144624$$

$$\mathbf{Ch(Sz_p},L_7) = x^7 - 1885x^5 - 52920x^4 - 610180x^3 - 3425400x^2 - 9134864x - 9207360$$

$$\mathbf{Ch(Sz_p},L_8) = x^8 - 4384x^6 - 195696x^5 - 3772704x^4 - 38064384x^3 - 205599168x^2 -$$

$$- 547395840x - 536544000$$

$$\mathbf{Ch(Sz_p},L_9) = x^9 - 9104x^7 - 609968x^6 - 18363979x^5 - 305573760x^4 - 2959776486x^3 -$$

$$- 16409667600x^2 - 47572507008x - 55285493760$$

$$\mathbf{Ch(Sz_p},L_{10}) = x^{10} - 17621x^8 - 1682384x^7 - 74094356x^6 - 1866611232x^5 -$$

$$- 28695471056x^4 - 270907003648x^3 - 1507725110272x^2 - 4422668451840x -$$

$$- 5049896140800$$

The characteristic polynomials of the $\mathbf{Sz}_p$ matrices, $\mathbf{Ch}(\mathbf{Sz}_p)$, for the rings R_3–R_{10} are:

$\mathbf{Ch}(\mathbf{Sz}_p,R_3) = x^3 - 3x - 2$

$\mathbf{Ch}(\mathbf{Sz}_p,R_4) = x^4 - 66x^2 - 128x - 63$

$\mathbf{Ch}(\mathbf{Sz}_p,R_5) = x^5 - 160x^3 - 1280x^2 - 3840x - 4096$

$\mathbf{Ch}(\mathbf{Sz}_p,R_6) = x^6 - 825x^4 - 11920x^3 - 67680x^2 - 174336x - 170240$

$\mathbf{Ch}(\mathbf{Sz}_p,R_7) = x^7 - 1701x^5 - 51030x^4 - 688905x^3 - 4960116x^2 - 18600435x - 28697814$

$\mathbf{Ch}(\mathbf{Sz}_p,R_8) = x^8 - 5068x^6 - 232848x^5 - 4779810x^4 - 54050976x^3 - 349963740x^2 -$

$- 1221605712x - 1789361847$

$\mathbf{Ch}(\mathbf{Sz}_p,R_9) = x^9 - 9216x^7 - 688128x^6 - 24772608x^5 - 528482304x^4 - 7046430720x^3 -$

$- 57982058496x^2 - 270582939648x - 549755813888$

$\mathbf{Ch}(\mathbf{Sz}_p,R_{10}) = x^{10} - 20745x^8 - 2163840x^7 - 107412480x^6 - 3172958208x^5 -$

$- 59935948800x^4 - 734967889920x^3 - 5686469591040x^2 - 25308094791680x -$

$- 49516677955584$

As is apparent from the above examples, all characteristic polynomials derived from the $\mathbf{Sz}_e$ and $\mathbf{Sz}_p$ matrices have large negative or positive values for their coefficients. This property makes them unsuitable for the computation of topological indices for structure-property models. The reciprocal Szeged matrix $\mathbf{RSz}_p$ has elements with lower values than those from the $\mathbf{Sz}_p$ matrix, giving polynomials with lower coefficients. The characteristic polynomials of the $\mathbf{RSz}_p$ matrices, $\mathbf{Ch}(\mathbf{RSz}_p)$, for the linear graphs L_3–L_{10} are presented below.

$\mathbf{Ch}(\mathbf{RSz}_p,L_3) = x^3 - 1.5x - 0.5$

$\mathbf{Ch}(\mathbf{RSz}_p,L_4) = x^4 - 0.84722x^2 - 0.33333x - 0.02194$

$\mathbf{Ch}(\mathbf{RSz}_p,L_5) = x^5 - 0.58333x^3 - 0.24537x^2 - 0.03318x - 0.00129$

$\mathbf{Ch}(\mathbf{RSz}_p,L_6) = x^6 - 0.41565x^4 - 0.15579x^3 - 0.01974x^2 - 0.00066x + 0.00001$

$\mathbf{Ch}(\mathbf{RSz}_p,L_7) = x^7 - 0.31676x^5 - 0.11019x^4 - 0.01430x^3 - 0.00069x^2$

$\mathbf{Ch}(\mathbf{RSz}_p,L_8) = x^8 - 0.24811x^6 - 0.07783x^5 - 0.00903x^4 - 0.00029x^3 + 0.00002x^2$

$\mathbf{Ch}(\mathbf{RSz}_p,L_9) = x^9 - 0.20106x^7 - 0.05817x^6 - 0.00639x^5 - 0.00020x^4 + 0.00002x^3$

$\mathbf{Ch}(\mathbf{RSz}_p,L_{10}) = x^{10} - 0.16599x^8 - 0.04399x^7 - 0.00435x^6 - 0.00008x^5 + 0.00002x^4$

The $\mathbf{Ch(RSz_p)}$ polynomial is a new polynomial in the family of polynomials with real value coefficients. In the above examples, the coefficients of the $\mathbf{Ch(RSz_p)}$ polynomials are presented with five decimal positions; the coefficients with an absolute value lower than 10^{-5} are not considered. The characteristic polynomials of the $\mathbf{RSz_p}$ matrices, $\mathbf{Ch(RSz_p)}$, for the rings R_3–R_{10} are given here.

$$\mathbf{Ch(RSz_p},R_3) = x^3 - 3x - 2$$

$$\mathbf{Ch(RSz_p},R_4) = x^4 - 2.25x^2 - 0.50x + 0.75$$

$$\mathbf{Ch(RSz_p},R_5) = x^5 - 0.62500x^3 - 0.31250x^2 - 0.05859x - 0.00391$$

$$\mathbf{Ch(RSz_p},R_6) = x^6 - 0.48611x^4 - 0.17361x^3 - 0.00651x^2 + 0.00477x + 0.00054$$

$$\mathbf{Ch(RSz_p},R_7) = x^7 - 0.25926x^5 - 0.09602x^4 - 0.01600x^3 - 0.00142x^2 - 0.00007x$$

$$\mathbf{Ch(RSz_p},R_8) = x^8 - 0.21065x^6 - 0.06361x^5 - 0.00700x^4 - 0.00009x^3 + 0.00005x^2$$

$$\mathbf{Ch(RSz_p},R_9) = x^9 - 0.14062x^7 - 0.04102x^6 - 0.00577x^5 - 0.00048x^4 + 0.00003x^3$$

$$\mathbf{Ch(RSz_p},R_{10}) = x^{10} - 0.11813x^8 - 0.02977x^7 - 0.00331x^6 - 0.00017x^5$$

The above examples demonstrate that, for the same molecular graph, the coefficients of the $\mathbf{Ch(RSz_p)}$ polynomials have much lower absolute values than those of the $\mathbf{Ch(Sz_e)}$ and $\mathbf{Ch(Sz_p)}$ polynomials. This property indicates that the $\mathbf{Ch(RSz_p)}$ polynomial is fit for the development of topological indices that can be used in structure-property or structure-biological activity studies.

The detour-distance matrix[34] is a first example of a nonsymmetric matrix; such a matrix contains much more information than the usual molecular symmetric matrix. We have to mention that many graph descriptors were developed from symmetric matrices and some of them cannot be computed from nonsymmetric matrices. The characteristic polynomial is an invariant for nonsymmetric matrices, and therefore it can be used for the nonsymmetric $\mathbf{Sz_u}$ and $\mathbf{RSz_u}$ Szeged matrices. The characteristic polynomials of the $\mathbf{Sz_u}$ matrices, $\mathbf{Ch(Sz_u)}$, for the linear graphs L_3-L_{10} are given below.

$$\mathbf{Ch(Sz_u},L_3) = x^3 - 5x - 4$$

$$\mathbf{Ch(Sz_u},L_4) = x^4 - 18x^2 - 40x - 24$$

$$\mathbf{Ch(Sz_u},L_5) = x^5 - 46x^3 - 202x^2 - 343x - 210$$

$$\mathbf{Ch(Sz_u},L_6) = x^6 - 101x^4 - 730x^3 - 2303x^2 - 3542x - 2205$$

$$\mathbf{Ch(Sz_u},L_7) = x^7 - 193x^5 - 2076x^4 - 10491x^3 - 29322x^2 - 44145x - 28350$$

$$\mathbf{Ch(Sz_u},L_8) = x^8 - 340x^6 - 5088x^5 - 37318x^4 - 161712x^3 - 424952x^2 - 633804x - 415800$$

$$\mathbf{Ch(Sz_u},L_9) = x^9 - 556x^7 - 11038x^6 - 110830x^5 - 686596x^4 - 2753420x^3 -$$

$$- 7037758x^2 - 10514127x - 7027020$$

$$\mathbf{Ch(Sz_u},L_{10}) = x^{10} - 865x^8 - 21992x^7 - 288940x^6 - 2410430x^5 - 13560710x^4 -$$

$$- 51837668x^3 - 130141701x^2 - 194618070x - 131756625$$

The characteristic polynomials of the $\mathbf{Sz_u}$ matrices, $\mathbf{Ch(Sz_u)}$, for the rings R_3–R_{10} are:

$\mathbf{Ch(Sz_u},R_3) = x^3 - 3x - 2$

$\mathbf{Ch(Sz_u},R_4) = x^4 - 18x^2 - 32x - 15$

$\mathbf{Ch(Sz_u},R_5) = x^5 - 40x^3 - 160x^2 - 240x - 128$

$\mathbf{Ch(Sz_u},R_6) = x^6 - 105x^4 - 680x^3 - 1800x^2 - 2208x - 1040$

$\mathbf{Ch(Sz_u},R_7) = x^7 - 189x^5 - 1890x^4 - 8505x^3 - 20412x^2 - 25515x - 13122$

$\mathbf{Ch(Sz_u},R_8) = x^8 - 364x^6 - 5040x^5 - 32130x^4 - 114912x^3 - 238140x^2 - 268272x - 127575$

$\mathbf{Ch(Sz_u},R_9) = x^9 - 576x^7 - 10752x^6 - 96768x^5 - 516096x^4 - 1720320x^3 - 3538944x^2 -$

$- 4128768x - 2097152$

$\mathbf{Ch(Sz_u},R_{10}) = x^{10} - 945x^8 - 22560x^7 - 262080x^6 - 1838592x^5 - 8332800x^4 -$

$- 24698880x^3 - 46448640x^2 - 50462720x - 24182784$

From these examples it is clear that polynomials derived from the $\mathbf{Sz_u}$ matrix have too large coefficients, and they are not of great use in deriving descriptors for QSPR and QSAR studies. On the other hand, $\mathbf{RSz_u}$ is a positive matrix with elements less or equal to unity that gives polynomials with lower coefficients. We present below the characteristic polynomials of the $\mathbf{RSz_u}$ matrices, $\mathbf{Ch(RSz_u)}$, for the linear graphs L_3–L_{10}.

$\mathbf{Ch(RSz_u},L_3) = x^3 - 2x - 1$

$\mathbf{Ch(RSz_u},L_4) = x^4 - 2.16667x^2 - 1.66667x - 0.35417$

$\mathbf{Ch(RSz_u},L_5) = x^5 - 2.33333x^3 - 2.30556x^2 - 0.86285x - 0.11343$

$\mathbf{Ch(RSz_u},L_6) = x^6 - 2.40000x^4 - 2.68889x^3 - 1.31630x^2 - 0.31370x - 0.02914$

$\mathbf{Ch(RSz_u},L_7) = x^7 - 2.46667x^5 - 3.04769x^4 - 1.77292x^3 - 0.57164x^2 - 0.09819x - 0.00691$

$\mathbf{Ch(RSz_u},L_8) = x^8 - 2.50238x^6 - 3.29258x^5 - 2.14818x^4 - 0.83877x^3 - 0.19904x^2 -$

$- 0.02629x - 0.00146$

$\mathbf{Ch(RSz_u},L_9) = x^9 - 2.53810x^7 - 3.52354x^6 - 2.51252x^5 - 1.12327x^4 - 0.32808x^3 -$

$- 0.06066x^2 - 0.00638x - 0.00029$

$\mathbf{Ch(RSz_u},L_{10}) = x^{10} - 2.56032x^8 - 3.69423x^7 - 2.81498x^6 - 1.39256x^5 - 0.47204x^4 -$

$- 0.10886x^3 - 0.01621x^2 - 0.00139x - 0.00005$

We give below the characteristic polynomials of the $\mathbf{RSz_u}$ matrices, $\mathbf{Ch(RSz_u)}$, for the rings R_3–R_{10}.

$$\mathbf{Ch(RSz_u},R_3) = x^3 - 3x - 2$$

$$\mathbf{Ch(RSz_u},R_4) = x^4 - 3x^2 - 2x$$

$$\mathbf{Ch(RSz_u},R_5) = x^5 - 2.50000x^3 - 2.50000x^2 - 0.93750x - 0.12500$$

$$\mathbf{Ch(RSz_u},R_6) = x^6 - 2.50000x^4 - 2.50000x^3 - 0.93750x^2 - 0.12500x$$

$$\mathbf{Ch(RSz_u},R_7) = x^7 - 2.33333x^5 - 2.59259x^4 - 1.29630x^3 - 0.34568x^2 - 0.04801x - 0.00274$$

$$\mathbf{Ch(RSz_u},R_8) = x^8 - 2.33333x^6 - 2.59259x^5 - 1.29630x^4 - 0.34568x^3 - 0.04801x^2 - 0.00274x$$

$$\mathbf{Ch(RSz_u},R_9) = x^9 - 2.25000x^7 - 2.62500x^6 - 1.47656x^5 - 0.49219x^4 - 0.10254x^3 -$$

$$- 0.01318x^2 - 0.00096x - 0.00003$$

$$\mathbf{Ch(RSz_u},R_{10}) = x^{10} - 2.25000x^8 - 2.62500x^7 - 1.47656x^6 - 0.49219x^5 - 0.10254x^4 -$$

$$- 0.01318x^3 - 0.00096x^2 - 0.00003x$$

For rings, this polynomial has an interesting property: if n is odd, $\mathbf{Ch(RSz_u},R_{n+1}) = x\mathbf{Ch(RSz_u},R_n)$. Similarly with the $\mathbf{Ch(RSz_p)}$ polynomial, the examples presented here show that the coefficients of the $\mathbf{Ch(RSz_u)}$ polynomial have much lower absolute values than those of the $\mathbf{Ch(Sz_e)}$ and $\mathbf{Ch(Sz_p)}$ polynomials. Therefore, this polynomial can be used to derive useful structural descriptors.

An eigenvalue x_i of the molecular matrix $\mathbf{M} = \mathbf{M}(G)$ is a zero of its characteristic polynomial, $\mathbf{Ch}(\mathbf{M},G,x_i) = 0$, for $i = 1$ to N. The complete set of graph eigenvalues $x_1, x_2, \ldots, x_N$ forms the spectrum of the molecular matrix $\mathbf{M}$, $\mathbf{Sp}(\mathbf{M},G) = \{x_i, i = 1, 2, \ldots, N\}$. The $\mathbf{Sp(Sz_e)}$ spectra of some linear and cyclic molecular graphs are presented below:

$$\mathbf{Sp(Sz_e},L_3) = \{2.82843, 0, -2.82843\}$$

$$\mathbf{Sp(Sz_e},L_4) = \{5.60555, 1.60555, -1.60555, -5.60555\}$$

$$\mathbf{Sp(Sz_e},L_5) = \{9.38083, 4, 0, -4, -9.38083\}$$

$$\mathbf{Sp(Sz_e},L_6) = \{14.16245, 7.32989, 2.16744, -2.16744, -7.32989, -14.16245\}$$

$$\mathbf{Sp(Sz_e},L_7) = \{19.94859, 11.66190, 5.10429, 0, -5.10429, -11.66190, -19.94859\}$$

$$\mathbf{Sp(Sz_e},L_8) = \{26.73722, 17.00887, 8.97332, 2.70168, -2.70168, -8.97332, -17.00887, -26.73722\}$$

$$\mathbf{Sp(Sz_e},L_9) = \{34.52721, 23.36715, 13.85179, 6.16250, 0, -6.16250, -13.85179,$$

$$-23.36715, -34.52721\}$$

$$\mathbf{Sp(Sz_e},L_9) = \{43.31799, 30.73220, 19.75546, 10.55752, 3.21627, -3.21627,$$

$$-10.55752, -19.75546, -30.73220, -43.31799\}$$

$\mathbf{Sp}(\mathbf{Sz}_e,R_3) = \{2, -1, -1\}$

$\mathbf{Sp}(\mathbf{Sz}_e,R_4) = \{8, 0, 0, -8\}$

$\mathbf{Sp}(\mathbf{Sz}_e,R_5) = \{8, 2.47214, 2.47214, -6.47214, -6.47214\}$

$\mathbf{Sp}(\mathbf{Sz}_e,R_6) = \{18, 9, 9, -9, -9, -18\}$

$\mathbf{Sp}(\mathbf{Sz}_e,R_7) = \{18, 11.22282, 11.22282, -4.00538, -4.00538, -16.21744, -16.21744\}$

$\mathbf{Sp}(\mathbf{Sz}_e,R_8) = \{32, 22.62742, 22.62742, 0, 0, -22.62742, -22.62742, -32\}$

$\mathbf{Sp}(\mathbf{Sz}_e,R_9) = \{32, 24.51342, 24.51342, 5.55674, 5.55674, -16, -16, -30.07016, -30.07016\}$

$\mathbf{Sp}(\mathbf{Sz}_e,R_{10}) = \{50, 40.45085, 40.45085, 15.45085, 15.45085, -15.45085, -15.45085, -40.45085,$

$-40.45085, -50\}$

The spectrum $\mathbf{Sp}(\mathbf{M},G)$ of the molecular graph matrix $\mathbf{M} = \mathbf{M}(G)$ is used to define two molecular descriptors, namely the maximum spectrum value, **MaxSp**, and the minimum spectrum value, **MinSp**:

$$\mathbf{MaxSp} = \max(\mathbf{Sp}(\mathbf{M},G)) \tag{15}$$

$$\mathbf{MinSp} = \min(\mathbf{Sp}(\mathbf{M},G)) \tag{16}$$

From the examples presented above one can see that for linear graphs **MaxSp** = –**MinSp**, while for rings R_n this property holds only when n is even. The spectra of linear graphs and those of rings R_n with n even are symmetric with respect to zero. Because the spectra $\mathbf{Sp}(\mathbf{Sz}_e)$ do not increase too quickly with the increase of the number of atoms in the molecular graph, they can generate useful structural descriptors. The spectra of the $\mathbf{Sz}_p$ matrices, $\mathbf{Sp}(\mathbf{Sz}_p)$, for the linear graphs L_3–L_{10} and the rings R_3–R_{10} are:

$\mathbf{Sp}(\mathbf{Sz}_p,L_3) = \{3.37228, -1, -2.37228\}$

$\mathbf{Sp}(\mathbf{Sz}_p,L_4) = \{9, -1, -3, -5\}$

$\mathbf{Sp}(\mathbf{Sz}_p,L_5) = \{18.47367, -2, -2.41952, -6, -8.05415\}$

$\mathbf{Sp}(\mathbf{Sz}_p,L_6) = \{33.70984, -1.60336, -4.07566, -5.10648, -9.78493, -13.13941\}$

$\mathbf{Sp}(\mathbf{Sz}_p,L_7) = \{55.33413, -2.90129, -3.57229, -7.45541, -7.49220, -16.64330, -17.26963\}$

$\mathbf{Sp}(\mathbf{Sz}_p,L_8) = \{85.23377, -2.21532, -5.47729, -7.85915, -10.27461, -11.15931,$

$-21.62487, -26.62324\}$

$\mathbf{Sp}(\mathbf{Sz}_p,L_9) = \{124.04750, -3.71292, -4.70106, -10.57412, -10.65248, -14.64097,$

$-14.73559, -29.95837, -35.07199\}$

$\mathbf{Sp}(\mathbf{Sz}_p, L_{10})$ = {173.65460, –2.84983, –6.75348, –10.61308, –13.75493, –16, –18.72221, –19.19168, –36.66062, –49.10876}

$\mathbf{Sp}(\mathbf{Sz}_p, R_3)$ = {2, –1, –1}

$\mathbf{Sp}(\mathbf{Sz}_p, R_4)$ = {9, –1, –1, –7}

$\mathbf{Sp}(\mathbf{Sz}_p, R_5)$ = {16, –4, –4, –4, –4}

$\mathbf{Sp}(\mathbf{Sz}_p, R_6)$ = {35, –4, –4, –4, –4, –19}

$\mathbf{Sp}(\mathbf{Sz}_p, R_7)$ = {54, –9, –9, –9, –9, –9, –9}

$\mathbf{Sp}(\mathbf{Sz}_p, R_8)$ = {91, –9, –9, –9, –9, –9, –9, –37}

$\mathbf{Sp}(\mathbf{Sz}_p, R_9)$ = {128, –16, –16, –16, –16, –16, –16, –16, –16}

$\mathbf{Sp}(\mathbf{Sz}_p, R_{10})$ = {189, –16, –16, –16, –16, –16, –16, –16, –16, –61}

While the $\mathbf{Sp}(\mathbf{Sz}_p)$ spectra of linear graphs have real number values, those of the rings have integer number values. Also, we have to point that the R_n spectra show degenerate values, e.g. for R_{10} the eigenvalue –16 is eight-times degenerated. The spectra of the $\mathbf{RSz}_p$ matrices, $\mathbf{Sp}(\mathbf{RSz}_p)$, for the linear graphs L_3–L_{10} and the rings R_3–R_{10} are presented below.

$\mathbf{Sp}(\mathbf{RSz}_p, L_3)$ = {1.36603, –0.36603, –1}

$\mathbf{Sp}(\mathbf{RSz}_p, L_4)$ = {1.08333, –0.08333, –0.41667, –0.58333}

$\mathbf{Sp}(\mathbf{RSz}_p, L_5)$ = {0.93994, –0.06583, –0.16667, –0.33333, –0.37411}

$\mathbf{Sp}(\mathbf{RSz}_p, L_6)$ = {0.80129, 0.01419, –0.09193, –0.18036, –0.25559, –0.28760}

$\mathbf{Sp}(\mathbf{RSz}_p, L_7)$ = {0.70893, 0.00961, –0.01990, –0.12768, –0.13016, –0.21526, –0.22554}

$\mathbf{Sp}(\mathbf{RSz}_p, L_8)$ = {0.62904, 0.05480, –0.02533, –0.07932, –0.09882, –0.10939, –0.18065, –0.19033}

$\mathbf{Sp}(\mathbf{RSz}_p, L_9)$ = {0.56914, 0.05973, –0.00754, –0.06269, –0.06355, –0.08693, –0.08761, –0.15925, –0.16130}

$\mathbf{Sp}(\mathbf{RSz}_p, L_{10})$ = {0.51725, 0.07530, –0.01018, –0.04666, –0.05045, –0.05240, –0.07327, –0.07741, –0.13945, –0.14274}

$\mathbf{Sp}(\mathbf{RSz}_p, R_3)$ = {2, –1, –1}

$\mathbf{Sp}(\mathbf{RSz}_p, R_4)$ = {1.5, 0.5, –1, –1}

$\mathbf{Sp(RSz_p},R_5) = \{1, -0.25, -0.25, -0.25, -0.25\}$

$\mathbf{Sp(RSz_p},R_6) = \{0.83333, 0.16667, -0.25, -0.25, -0.25, -0.25\}$

$\mathbf{Sp(RSz_p},R_7) = \{0.66667, -0.11111, -0.11111, -0.11111, -0.11111, -0.11111, -0.11111\}$

$\mathbf{Sp(RSz_p},R_8) = \{0.58333, 0.08333, -0.11111, -0.11111, -0.11111, -0.11111, -0.11111, -0.11111\}$

$\mathbf{Sp(RSz_p},R_9) = \{0.5, -0.06250, -0.06250, -0.06250, -0.06250, -0.06250, -0.06250, -0.06250, -0.06250\}$

$\mathbf{Sp(RSz_p},R_{10}) = \{0.45, 0.05, -0.06250, -0.06250, -0.06250, -0.06250, -0.06250, -0.06250, -0.06250, -0.06250\}$

The $\mathbf{Sp(RSz_p)}$ spectra of both linear graphs and rings have real number values. When n increases, **MinSp** increases and **MaxSp** decreases; therefore, for the $\mathbf{Sp(RSz_p)}$ spectra the two descriptors do not reflect the size but the molecular shape. The $\mathbf{Sp(RSz_p)}$ spectra for rings show degenerate values, e.g. for R_{10} the eigenvalue –0.06250 is eight-times degenerated. The results reported in this section show that the spectra of the $\mathbf{Sz_e}$, $\mathbf{Sz_p}$, and $\mathbf{RSz_p}$ matrices can be used to generate new structural descriptors.

THE HOSOYA OPERATOR FOR SZEGED MATRICES

For a graph G with N vertices the Hosoya operator $\mathbf{Ho(M)} = \mathbf{Ho(M},G)$ is defined as the sum of the absolute values of the coefficients of the characteristic polynomial of the matrix **M**:[33]

$$\mathbf{Ho(M)} = \sum_{n=0}^{N} |c_n| . \tag{17}$$

For alkanes and if **M** is the adjacency matrix **A** the **Ho** operator is identical with the Hosoya index Z.[12] From the definition of the Hosoya operator it is obvious that it can be applied both to symmetric and nonsymmetric matrices. Some values of the Hosoya operator for the $\mathbf{Sz_e}$ and $\mathbf{Sz_p}$ matrices are presented below.

$\mathbf{Ho(Sz_e},L_3) = 9$

$\mathbf{Ho(Sz_e},L_4) = 116$

$\mathbf{Ho(Sz_e},L_5) = 1513$

$\mathbf{Ho(Sz_e},L_6) = 62856$

$\mathbf{Ho(Sz_e},L_7) = 1478641$

$\mathbf{Ho(Sz_e},L_8) = 140599952$

$\mathbf{Ho(Sz_e},L_9) = 4906409841$

$\mathbf{Ho(Sz_e},L_{10}) = 886104141344$

$\mathbf{Ho(Sz_e},R_3) = 6$

$\mathbf{Ho(Sz_e},R_4) = 65$

$\mathbf{Ho(Sz_e},R_5) = 3409$

$\mathbf{Ho(Sz_e},R_6) = 2185300$

$\mathbf{Ho(Sz_e},R_7) = 13378447$

$\mathbf{Ho(Sz_e},R_8) = 269748225$

$\mathbf{Ho(Sz_e},R_9) = 176598747393$

$\mathbf{Ho(Sz_e},R_{10}) = 385296644537501$

$\mathbf{Ho(Sz_p},L_3) = 18$ $\mathbf{Ho(Sz_p},L_4) = 386$

$\mathbf{Ho(Sz_p},L_5) = 11363$ $\mathbf{Ho(Sz_p},L_6) = 402482$

$\mathbf{Ho(Sz_p},L_7) = 22432610$ $\mathbf{Ho(Sz_p},L_8) = 1331576177$

$\mathbf{Ho(Sz_p},L_9) = 122552001666$ $\mathbf{Ho(Sz_p},L_{10}) = 11281834583210$

$\mathbf{Ho(Sz_p},R_3) = 6$ $\mathbf{Ho(Sz_p},R_4) = 258$

$\mathbf{Ho(Sz_p},R_5) = 9377$ $\mathbf{Ho(Sz_p},R_6) = 425002$

$\mathbf{Ho(Sz_p},R_7) = 53000002$ $\mathbf{Ho(Sz_p},R_8) = 3420000002$

$\mathbf{Ho(Sz_p},R_9) = 885921195009$ $\mathbf{Ho(Sz_p},R_{10}) = 81309428732298$

From these examples it is clear that the Hosoya operator **Ho** derived from the $\mathbf{Sz_e}$ and $\mathbf{Sz_p}$ matrices have too large values, and they are not of great use in deriving descriptors for QSPR and QSAR studies. However, with a proper scaling down, e.g. by logarithmation, they can be of certain interest. The values of the Hosoya operator for the $\mathbf{RSz_p}$ matrix, obtained from the coefficients of the polynomials $\mathbf{Ch(RSz_p},L_n)$ and $\mathbf{Ch(RSz_p},R_n)$ are:

$\mathbf{Ho(RSz_p},L_3) = 3\mathbf{Ho}$ $\mathbf{(RSz_p},L_4) = 2.20250$

$\mathbf{Ho(RSz_p},L_5) = 1.86317$ $\mathbf{Ho(RSz_p},L_6) = 1.59185$

$\mathbf{Ho(RSz_p},L_7) = 1.44194$ $\mathbf{Ho(RSz_p},L_8) = 1.33528$

$\mathbf{Ho(RSz_p},L_9) = 1.26584$ $\mathbf{Ho(RSz_p},L_{10}) = 1.21443$

$\mathbf{Ho(RSz_p},R_3) = 6$ $\mathbf{Ho(RSz_p},R_4) = 4.5$

$\mathbf{Ho(RSz_p},R_5) = 2$ $\mathbf{Ho(RSz_p},R_6) = 1.67155$

$\mathbf{Ho(RSz_p},R_7) = 1.37277$ $\mathbf{Ho(RSz_p},R_8) = 1.28140$

$\mathbf{Ho(RSz_p},R_9) = 1.18791$ $\mathbf{Ho(RSz_p},R_{10}) = 1.15137$

The $\mathbf{Ho(RSz_p)}$ descriptors do not reflect the molecular size, i.e. they decrease when the number of atoms in the molecular graph increases. The Hosoya operator applied to the nonsymmetric $\mathbf{Sz_u}$ and $\mathbf{RSz_u}$ matrices gives the following descriptors:

$\mathbf{Ho(Sz_u},L_3) = 10$ $\mathbf{Ho(Sz_u},L_4) = 83$

$\mathbf{Ho(Sz_u},L_5) = 802$ $\mathbf{Ho(Sz_u},L_6) = 8882$

$\mathbf{Ho(Sz_u},L_7) = 114578$ $\mathbf{Ho(Sz_u},L_8) = 1679015$

$\mathbf{Ho(Sz_u},L_9) = 28141346$ $\mathbf{Ho(Sz_u},L_{10}) = 524637002$

$\mathbf{Ho(Sz_u},R_3) = 6$ $\mathbf{Ho(Sz_u},R_4) = 66$

$\mathbf{Ho(Sz_u},R_5) = 569$ $\mathbf{Ho(Sz_u},R_6) = 5834$

$\mathbf{Ho(Sz_u},R_7) = 69634$ $\mathbf{Ho(Sz_u},R_8) = 786434$

$\mathbf{Ho(Sz_u},R_9) = 12109377$ $\mathbf{Ho(Sz_u},R_{10}) = 156250002$

$\mathbf{Ho(RSz_u},L_3) = 4$ $\mathbf{Ho(RSz_u},L_4) = 5.18750$

$\mathbf{Ho(RSz_u},L_5) = 6.61516$ $\mathbf{Ho(RSz_u},L_6) = 7.74803$

$\mathbf{Ho(RSz_u},L_7) = 8.96401$ $\mathbf{Ho(RSz_u},L_8) = 10.00870$

$\mathbf{Ho(RSz_u},L_9) = 11.09283$ $\mathbf{Ho(RSz_u},L_{10}) = 12.06064$

$\mathbf{Ho(RSz_u},R_3) = 6$ $\mathbf{Ho(RSz_u},R_4) = 6$

$\mathbf{Ho(RSz_u},R_5) = 7.06250$ $\mathbf{Ho(RSz_u},R_6) = 7.06250$

$\mathbf{Ho(RSz_u},R_7) = 7.61866$ $\mathbf{Ho(RSz_u},R_8) = 7.61866$

$\mathbf{Ho(RSz_u},R_9) = 7.96046$ $\mathbf{Ho(RSz_u},R_{10}) = 7.96046$

An interesting property is exhibited for the Hosoya indices of rings: if n is odd, $\mathbf{Ho(RSz_u},R_n) = \mathbf{Ho(RSz_u},R_{n+1})$. From these examples it is clear that Hosoya descriptors derived from the $\mathbf{Sz_u}$ matrix have too large values, while those obtained from the $\mathbf{RSz_u}$ matrix increase slowly when the number of atoms in the molecular graph increases.

SPECTRAL MOMENTS DERIVED FROM THE SZEGED MATRICES

Another molecular graph invariant that can be computed both for symmetric and nonsymmetric matrices is the spectral moment. The spectral moment of order k of the molecular matrix $\mathbf{M} = \mathbf{M}(G)$, $\mathbf{SM(M)}_k$, is defined as:[2,3,5]

$$\mathbf{SM}(k,\mathbf{M}) = \sum_{i=1}^{N} x_i^k = \mathbf{TrM}^k \tag{18}$$

where the trace of the kth power of the molecular matrix $\mathbf{M}$ is equal to:

$$\mathbf{TrM}^k = \sum_{i=1}^{N} [\mathbf{M}^k]_{ii}. \tag{19}$$

In this paper we will give some examples of spectral moments computed from the Szeged matrices. For each molecule we present the **SM** up to the sixth power, i.e. for k from 1 to 6. We have to mention that for a molecular graph with N vertices, the first N spectral moments can be used to compute the characteristic polynomial.[2,3,5] The first six spectral moments of the $\mathbf{Sz_e}$ matrices, $\mathbf{SM(Sz_e)}$, for the

linear graphs L_3–L_{10} and the rings R_3–R_{10} are presented below.

$\mathbf{SM(Sz_e},L_3) = \{0, 16, 0, 128, 0, 1024\}$

$\mathbf{SM(Sz_e},L_4) = \{0, 68, 0, 1988, 0, 62084\}$

$\mathbf{SM(Sz_e},L_5) = \{0, 208, 0, 16000, 0, 1371136\}$

$\mathbf{SM(Sz_e},L_6) = \{0, 518, 0, 86278, 0, 16448774\}$

$\mathbf{SM(Sz_e},L_7) = \{0, 1120, 0, 355072, 0, 131104768\}$

$\mathbf{SM(Sz_e},L_8) = \{0, 2184, 0, 1202568, 0, 780151560\}$

$\mathbf{SM(Sz_e},L_9) = \{0, 3936, 0, 3515136, 0, 3728252928\}$

$\mathbf{SM(Sz_e},L_{10}) = \{0, 6666, 0, 9155850, 0, 15020794122\}$

$\mathbf{SM(Sz_e},R_3) = \{0, 6, 6, 18, 30, 66\}$

$\mathbf{SM(Sz_e},R_4) = \{0, 128, 0, 8192, 0, 524288\}$

$\mathbf{SM(Sz_e},R_5) = \{0, 160, 0, 7680, 10240, 409600\}$

$\mathbf{SM(Sz_e},R_6) = \{0, 972, 0, 236196, 0, 70150212\}$

$\mathbf{SM(Sz_e},R_7) = \{0, 1134, 0, 275562, 0, 74401740\}$

$\mathbf{SM(Sz_e},R_8) = \{0, 4096, 0, 3145728, 0, 2684354560\}$

$\mathbf{SM(Sz_e},R_9) = \{0, 4608, 0, 3538944, 0, 3019898880\}$

$\mathbf{SM(Sz_e},R_{10}) = \{0, 12500, 0, 23437500, 0, 48828125000\}$

From these examples one can see that the odd spectral moments $\mathbf{SM(Sz_e)}$ are zero in linear graphs. The spectral moments of the $\mathbf{Sz_e}$ matrix, $\mathbf{SM(Sz_e)}_k$, increase very quickly with the increase of k and of the number of atoms in the molecular graph. This trend is also exhibited by the spectral moments of the $\mathbf{Sz_p}$ matrices, $\mathbf{SM(Sz_p)}$; their first six spectral moments for the graphs L_3–L_{10} and R_3–R_{10} are given below.

$\mathbf{SM(Sz_p},L_3) = \{0, 18, 24, 162, 360, 1650\}$

$\mathbf{SM(Sz_p},L_4) = \{0, 116, 576, 7268, 55680, 547796\}$

$\mathbf{SM(Sz_p},L_5) = \{0, 452, 5544, 122024, 2109840, 40068272\}$

$\mathbf{SM(Sz_p},L_6) = \{0, 1450, 34896, 1331234, 43043520, 1473416866\}$

$\mathbf{SM(Sz_p},L_7) = \{0, 3770, 158760, 9547170, 515898000, 28753182434\}$

$\mathbf{SM(Sz_p},L_8) = \{0, 8768, 587088, 53529728, 4479978240, 383877764480\}$

$\mathbf{SM(Sz_p},L_9) = \{0, 18208, 1829904, 239221548, 29293612160, 3646185844612\}$

$\mathbf{SM(Sz_p},L_{10}) = \{0, 35242, 5047152, 917376706, 157559498480, 27439748827282\}$

$\mathbf{SM}(\mathbf{Sz_p},R_3)$ = {0, 6, 6, 18, 30, 66}

$\mathbf{SM}(\mathbf{Sz_p},R_4)$ = {0, 132, 384, 8964, 42240, 649092}

$\mathbf{SM}(\mathbf{Sz_p},R_5)$ = {0, 320, 3840, 66560, 1044480, 16793600}

$\mathbf{SM}(\mathbf{Sz_p},R_6)$ = {0, 1650, 35760, 1631970, 50041680, 1885327890}

$\mathbf{SM}(\mathbf{Sz_p},R_7)$ = {0, 3402, 153090, 8542422, 458810730, 24798099942}

$\mathbf{SM}(\mathbf{Sz_p},R_8)$ = {0, 10136, 698544, 70488488, 6170623200, 570438167096}

$\mathbf{SM}(\mathbf{Sz_p},R_9)$ = {0, 18432, 2064384, 268959744, 34351349760, 4398180728832}

$\mathbf{SM}(\mathbf{Sz_p},R_{10})$ = {0, 41490, 6491520, 1290359970, 240309095040, 45631287702450}

Because the spectral moments of the $\mathbf{Sz_p}$ matrix have too large values, we have investigated the reciprocal matrix $\mathbf{RSz_p}$; this is a positive matrix with elements less or equal to unity that can generate spectral moments with lower values, compared with those obtained from $\mathbf{Sz_p}$. The first six spectral moments $\mathbf{SM}(\mathbf{RSz_p})$ for graphs L_3–L_{10} and R_3–R_{10} are presented below.

$\mathbf{SM}(\mathbf{RSz_p},L_3)$ = {0, 3, 1.5, 4.5, 3.75, 7.5, 7.87500, 13.12500, 15.56250, 23.62500}

$\mathbf{SM}(\mathbf{RSz_p},L_4)$ = {0, 1.69444, 1.00000, 1.52334, 1.41204, 1.66112, 1.72603, 1.91144, 2.04702, 2.23121}

$\mathbf{SM}(\mathbf{RSz_p},L_5)$ = {0, 1.16667, 0.73611, 0.81327, 0.72209, 0.69374, 0.64670, 0.60979, 0.57247, 0.53834}

$\mathbf{SM}(\mathbf{RSz_p},L_6)$ = {0, 0.83130, 0.46736, 0.42449, 0.32708, 0.26558, 0.21186, 0.17002, 0.13617, 0.10913}

$\mathbf{SM}(\mathbf{RSz_p},L_7)$ = {0, 0.63352, 0.33056, 0.25788, 0.17795, 0.12719, 0.08994, 0.06381, 0.04523, 0.03207}

$\mathbf{SM}(\mathbf{RSz_p},L_8)$ = {0, 0.49622, 0.23349, 0.15923, 0.09802, 0.06204, 0.03895, 0.02452, 0.01542, 0.00970}

$\mathbf{SM}(\mathbf{RSz_p},L_9)$ = {0, 0.40212, 0.17450, 0.10641, 0.05949, 0.03402, 0.01934, 0.01101, 0.00627, 0.00357}

$\mathbf{SM}(\mathbf{RSz_p},L_{10})$ = {0, 0.33197, 0.13197, 0.07249, 0.03691, 0.01917, 0.00990, 0.00512, 0.00265, 0.00137}

$\mathbf{SM(RSz_p},R_3) = \{0, 6, 6, 18, 30, 66, 126, 258, 510, 1026\}$

$\mathbf{SM(RSz_p},R_4) = \{0, 4.50000, 1.50000, 7.12500, 5.62500, 13.40625, 15.09375, 27.63281, 36.44531, 59.66602\}$

$\mathbf{SM(RSz_p},R_5) = \{0, 1.25000, 0.93750, 1.01562, 0.99609, 1.00098, 0.99976, 1.00006, 0.99998, 1.00000\}$

$\mathbf{SM(RSz_p},R_6) = \{0, 0.97222, 0.52083, 0.49865, 0.39810, 0.33590, 0.27884, 0.23263, 0.19379, 0.16151\}$

$\mathbf{SM(RSz_p},R_7) = \{0, 0.51852, 0.28807, 0.19845, 0.13159, 0.08780, 0.05853, 0.03902, 0.02601, 0.01734\}$

$\mathbf{SM(RSz_p},R_8) = \{0, 0.42130, 0.19084, 0.11675, 0.06745, 0.03941, 0.02298, 0.01341, 0.00782, 0.00456\}$

$\mathbf{SM(RSz_p},R_9) = \{0, 0.28125, 0.12305, 0.06262, 0.03124, 0.01563, 0.00781, 0.00391, 0.00195, 0.00098\}$

$\mathbf{SM(RSz_p},R_{10}) = \{0, 0.23625, 0.08930, 0.04113, 0.01845, 0.00830, 0.00374, 0.00168, 0.00076, 0.00034\}$

The spectral moments of the $\mathbf{RSz_p}$ matrix, $\mathbf{SM(RSz_p)}_k$, decrease with the increase of k and of the number of atoms in the molecular graph. This property shows that these spectral moments are not correlated with the molecular size, and the descriptors derived from them cannot be used in monoparametric equations to correlate size-dependent molecular properties. We continue the analysis of the spectral moments derived from Szeged matrices with $\mathbf{SM(Sz_u)}$ spectral moments.

$\mathbf{SM(Sz_u},L_3) = \{0, 10, 12, 50, 100, 298\}$

$\mathbf{SM(Sz_u},L_4) = \{0, 36, 120, 744, 3600, 19056\}$

$\mathbf{SM(Sz_u},L_5) = \{0, 92, 606, 5604, 47510, 411752\}$

$\mathbf{SM(Sz_u},L_6) = \{0, 202, 2190, 29614, 386360, 5068150\}$

$\mathbf{SM(Sz_u},L_7) = \{0, 386, 6228, 116462, 2149950, 39720890\}$

$\mathbf{SM(Sz_u},L_8) = \{0, 680, 15264, 380472, 9458160, 234949664\}$

$\mathbf{SM(Sz_u},L_9) = \{0, 1112, 33114, 1061592, 34118620, 1095520964\}$

$\mathbf{SM(Sz_u},L_{10}) = \{0, 1730, 65976, 2652210, 107167550, 4326336302\}$

$\mathbf{SM}(\mathbf{Sz_u},R_3)$ = {0, 6, 6, 18, 30, 66}

$\mathbf{SM}(\mathbf{Sz_u},R_4)$ = {0, 36, 96, 708, 2880, 16356}

$\mathbf{SM}(\mathbf{Sz_u},R_5)$ = {0, 80, 480, 4160, 32640, 262400}

$\mathbf{SM}(\mathbf{Sz_u},R_6)$ = {0, 210, 2040, 29250, 368040, 4842690}

$\mathbf{SM}(\mathbf{Sz_u},R_7)$ = {0, 378, 5670, 105462, 1888110, 34016598}

$\mathbf{SM}(\mathbf{Sz_u},R_8)$ = {0, 728, 15120, 393512, 9747360, 244262648}

$\mathbf{SM}(\mathbf{Sz_u},R_9)$ = {0, 1152, 32256, 1050624, 33546240, 1073774592}

$\mathbf{SM}(\mathbf{Sz_u},R_{10})$ = {0, 1890, 67680, 2834370, 115788960, 4750668450}

For the same molecular graph, the elements of the $\mathbf{Sz_u}$ matrix have lower values than those of the $\mathbf{Sz_p}$ matrix; although the $\mathbf{SM}(\mathbf{Sz_u})_k$ spectral moments increase with the increase of k and of the number of atoms in the molecular graph, they increase at a lower rate than the $\mathbf{SM}(\mathbf{Sz_e})$ and $\mathbf{SM}(\mathbf{Sz_p})$ spectral moments. We investigate now the trend of the $\mathbf{SM}(\mathbf{RSz_u})$ spectral moments.

$\mathbf{SM}(\mathbf{RSz_u},L_3)$ = {0, 4, 3, 8, 10, 19, 28, 48, 75, 124}

$\mathbf{SM}(\mathbf{RSz_u},L_4)$ = {0, 4.33333, 5.00000, 10.80556, 18.05556, 33.28009, 58.90046, 106.02643, 189.47917, 339.67806}

$\mathbf{SM}(\mathbf{RSz_u},L_5)$ = {0, 4.66667, 6.91667, 14.34028, 27.46528, 53.43403, 103.64530, 201.16012, 390.35906, 757.55429}

$\mathbf{SM}(\mathbf{RSz_u},L_6)$ = {0, 4.80000, 8.06667, 16.78519, 33.83519, 68.46787, 138.46184, 280.06664, 566.44869, 1145.69578}

$\mathbf{SM}(\mathbf{RSz_u},L_7)$ = {0, 4.93333, 9.14306, 19.26059, 40.44631, 84.71016, 177.54618, 372.07782, 779.76731, 1634.15655}

$\mathbf{SM}(\mathbf{RSz_u},L_8)$ = {0, 5.00476, 9.87774, 21.11655, 45.39027, 97.31027, 208.71269, 447.61360, 959.99654, 2058.88493}

$\mathbf{SM}(\mathbf{RSz_u},L_9)$ = {0, 5.07619, 10.57062, 22.93392, 50.33175, 110.17689, 241.24067, 528.19723, 1156.50309, 2532.19069}

$\mathbf{SM}(\mathbf{RSz_u},L_{10})$ = {0, 5.12063, 11.08268, 24.37038, 54.25472, 120.58458, 268.02930, 595.74627, 1324.17137, 2943.25025}

$\mathbf{SM}(\mathbf{RSz_u},R_3)$ = {0, 6, 6, 18, 30, 66, 126, 258, 510, 1026}

$\mathbf{SM}(\mathbf{RSz_u},R_4)$ = {0, 6, 6, 18, 30, 66, 126, 258, 510, 1026}

$\mathbf{SM}(\mathbf{RSz_u},R_5)$ = {0, 5.00000, 7.50000, 16.25000, 31.87500, 64.06250, 127.96875, 256.01562, 511.99219, 1024.00391}

$\mathbf{SM}(\mathbf{RSz_u},R_6)$ = {0, 5.00000, 7.50000, 16.25000, 31.87500, 64.06250, 127.96875, 256.01562, 511.99219, 1024.00391}

$\mathbf{SM}(\mathbf{RSz_u},R_7)$ = {0, 4.66667, 7.77778, 16.07407, 31.97531, 64.00823, 127.99726, 256.00091, 511.99970, 1024.00010}

$\mathbf{SM}(\mathbf{RSz_u},R_8)$ = {0, 4.66667, 7.77778, 16.07407, 31.97531, 64.00823, 127.99726, 256.00091, 511.99970, 1024.00010}

$\mathbf{SM}(\mathbf{RSz_u},R_9)$ = {0, 4.50000, 7.87500, 16.03125, 31.99219, 64.00195, 127.99951, 256.00012, 511.99997, 1024.00001}

$\mathbf{SM}(\mathbf{RSz_u},R_{10})$ = {0, 4.50000, 7.87500, 16.03125, 31.99219, 64.00195, 127.99951, 256.00012, 511.99997, 1024.00001}

Similarly with the $\mathbf{SM}(\mathbf{RSz_p})$ spectral moments, $\mathbf{SM}(\mathbf{RSz_p})_k$ decrease with the increase of k and of the number of atoms in the molecular graph. For rings, an interesting property is exhibited: for n odd, $\mathbf{SM}(\mathbf{RSz_u},R_n)_k = \mathbf{SM}(\mathbf{RSz_u},R_{n+1})_k$.

CONCLUSIONS

As a result of the considerable interest for structural descriptors, new topological indices were derived from Szeged matrices. In this paper we have investigated several graph descriptors derived from the symmetric ($\mathbf{Sz_e}$, $\mathbf{Sz_p}$, $\mathbf{RSz_p}$) and nonsymmetric ($\mathbf{Sz_u}$, $\mathbf{RSz_u}$) Szeged matrices: characteristic polynomials, matrix spectra, Hosoya indices, spectral moments. The graph invariants **Ch**, **Ho**, and **SM** derived from the $\mathbf{Sz_e}$, $\mathbf{Sz_p}$, and $\mathbf{Sz_u}$ matrices have too large values, and they are not of great use in deriving descriptors for structure-property models. However, with a proper scaling down, e.g. by logarithmation, they can be of certain interest. On the other hand, the graph invariants **Ch**, **Ho**, and **SM** computed from the $\mathbf{RSz_p}$, and $\mathbf{RSz_u}$ matrices have lower values; their use in QSPR and QSAR studies deserves further investigations. The **MinSp** and **MaxSp** descriptors of all Szeged matrices have interesting properties, making them interesting parameters for structure-property studies. Because the absolute values of **MinSp** and **MaxSp** descriptors derived from the $\mathbf{Sz_e}$, and $\mathbf{Sz_p}$ matrices do not increase too quickly with the increase of the number of atoms in the molecular graph, they can represent useful structural descriptors. On the other hand, the absolute values of **MinSp** and **MaxSp** descriptors derived from the $\mathbf{RSz_p}$ matrix decrease with the increase of the number of atoms in the molecular graph, showing that the two descriptors do not reflect the size but the molecular shape.

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