Cluj and Related Polynomials Applied in Correlating Studies[†]

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A counting polynomial $P(G,x)$ is a description of a graph property $P(G)$ in terms of a sequence of numbers so that the exponents express the extent of its partitions while the coefficients are related to the frequency of the occurrence of partitions. Basic definitions and properties of Cluj counting polynomials $CJ(G,x)$ and their relation with $\Omega(G,x)$ and $N\Omega(G,x)$ polynomials are presented. Analytical relations for the calculation of such polynomials and their single-number descriptors in some classes of planar polyhexes are derived. The ability of these descriptors to predict the boiling point, chromatographic retention index, and resonance energy for some planar polyhex compounds, as well as the toxicity of a set of dibenzofurans, is demonstrated.

1. INTRODUCTION

A graph $G(V,E)$, in which V is the set of vertices and E the set of its edges, can be described by a connection table, a sequence of numbers, a single number (called a topological index), a matrix, or a polynomial. Quantum chemistry was the first field that used the polynomial description of a molecular graph. In the early Hückel theory, the roots of the most studied *characteristic polynomial*[1,2]

$$P(G,x) = \det[x\mathbf{I} - \mathbf{A}(G)] \tag{1}$$

are related to the π-electron energy levels of the molecular orbitals in conjugated hydrocarbons. In eq 1, $\mathbf{I}$ is the unit matrix of a pertinent order and $\mathbf{A}$ the adjacency matrix of graph G. The characteristic polynomial is involved in the topological resonance energy, the topological effect on molecular orbitals, the aromatic sextet theory, and the Kekulé structure count.[1−5]

An extension of relation 1 was made by Hosoya et al.[6] and others[7,8] who changed the adjacency matrix by the distance matrix and, alternatively, by any square topological matrix.

The polynomial coefficients, $m(G,k)$, as presented in the equation

$$P(G,x) = \sum_k m(G,k)x^k \tag{2}$$

can be calculated from the graph by a method which makes use of the *Sachs graphs*, which are subgraphs of G. Equation 2 was derived independently by Sachs, Harary, Milić, Spialter, and Hosoya.[2] This method is useful with small graphs, but in larger graphs, the numeric methods of linear algebra, such as the recursive algorithms of Le Verier, Frame, or Fadeev, are more efficient.[9,10]

Equation 2 is a general expression of a counting polynomial, written as a sequence of numbers, with the exponents showing the extent of partitions $p(G)$, $\cup p(G) = P(G)$ of a graph property $P(G)$ while the coefficients $m(G,k)$ are related to the occurrence of partitions of extent k.

Counting polynomials were introduced in the mathematical chemistry literature by Hosoya[11,12] with his Z-counting (independent edge sets) and the distance degree (initially called Wiener and later Hosoya)[13,14] polynomials. Their roots and coefficients are used for the characterization of the topological nature of hydrocarbons.

Hosoya and Yamaguchi also proposed the sextet polynomial[15,16] for counting the resonant rings in a benzenoid molecule. The sextet polynomial is important in connection with the Clar aromatic sextets,[17,18] which are expected to stabilize the aromatic molecules.

The independence polynomial[19−21] counts the selections of k-independent vertices of G. Other related graph polynomials are the *king*, *color*, and *star polynomials*.[21−23]

If one counts sets of mutually adjacent vertices instead of the sets of independent vertices, one obtains the *clique polynomial*.[24] Polynomials are the subject of an extensive review.[1] For some distance-related properties, the polynomial coefficients are calculable from the layer and shell matrices,[25−29] which can be built according to the vertex distance partitions of a graph and are calculable by the TOPOCLUJ software package.[30]

This paper is focused on the mathematical aspects of the Cluj polynomials in relation to Ω-type polynomials, which could be a promise in the mathematical description of topology of various classes of molecules, with possible use in correlating studies. The definitions of Cluj matrices are provided in the next section; the Cluj polynomials are defined in the third section, and the properties of the Cluj and two related counting polynomials are presented in the fourth section. The final section presents several examples of the utility of descriptors derived from Cluj and related polynomials in the prediction of some physicochemical and biological properties of polycyclic structures.

CLUJ AND RELATED POLYNOMIALS

J. Chem. Inf. Model., Vol. 47, No. 3, 2007 **865**

Chart 1

UCJDI$_p$(DPH)

	1	2	3	4	5	6	7	8	9	10	11	12	RS
1	0	6	8	8	8	9	7	7	6	7	5	6	77
2	6	0	9	8	8	8	7	6	7	7	6	5	77
3	2	3	0	9	5	5	5	5	4	5	3	4	50
4	2	2	3	0	6	2	4	4	4	4	3	3	37
5	2	2	2	6	0	3	4	4	4	4	3	3	37
6	3	2	5	5	9	0	5	4	5	5	4	3	50
7	3	4	5	5	4	5	0	9	5	5	2	3	50
8	3	3	4	4	4	4	3	0	6	2	2	2	37
9	3	3	4	4	4	4	2	6	0	3	2	2	37
10	4	3	5	4	5	5	5	5	9	0	3	2	50
11	5	6	7	7	6	7	8	8	8	9	0	6	77
12	6	5	7	6	7	7	9	8	8	8	6	0	77
CS	39	39	59	66	66	59	59	66	66	59	39	39	656

UCJDI$_e$(DPH)

	1	2	3	4	5	6	7	8	9	10	11	12	RS
1	0	6	0	0	0	9	0	0	0	0	0	6	21
2	6	0	9	0	0	0	0	0	0	0	6	0	21
3	0	3	0	9	0	0	0	0	0	0	0	0	12
4	0	0	3	0	6	0	0	0	0	0	0	0	9
5	0	0	0	6	0	3	0	0	0	0	0	0	9
6	3	0	0	0	9	0	0	0	0	0	0	0	12
7	0	0	0	0	0	0	0	9	0	0	0	3	12
8	0	0	0	0	0	0	3	0	6	0	0	0	9
9	0	0	0	0	0	0	0	6	0	3	0	0	9
10	0	0	0	0	0	0	0	0	9	0	3	0	12
11	0	6	0	0	0	0	0	0	0	9	0	6	21
12	6	0	0	0	0	0	9	0	0	0	6	0	21
CS	15	15	12	15	15	12	12	15	15	12	15	15	168

UCJDE$_p$(DPH)

	1	2	3	4	5	6	7	8	9	10	11	12	RS
1	0	3	2	2	1	1	1	2	1	1	3	1	18
2	3	0	1	1	2	2	1	1	2	1	1	3	18
3	2	1	0	1	1	2	2	2	1	1	1	1	15
4	2	1	1	0	1	1	3	3	2	2	3	2	21
5	1	2	1	1	0	1	2	2	3	3	2	3	21
6	1	2	2	1	1	0	1	1	2	2	1	1	15
7	1	1	2	2	1	1	0	1	1	2	2	1	15
8	3	2	3	3	2	2	1	0	1	1	2	1	21
9	2	3	2	2	3	3	1	1	0	1	1	2	21
10	1	1	1	1	2	2	2	1	1	0	1	2	15
11	3	1	1	2	1	1	2	2	1	1	0	3	18
12	1	3	1	1	2	1	1	1	2	2	3	0	18
CS	20	20	17	17	17	17	17	17	17	17	20	20	216

UCJDE$_e$(DPH)

	1	2	3	4	5	6	7	8	9	10	11	12	RS
1	0	3	0	0	0	1	0	0	0	0	0	1	5
2	3	0	1	0	0	0	0	0	0	0	1	0	5
3	0	1	0	1	0	0	0	0	0	0	0	0	2
4	0	0	1	0	1	0	0	0	0	0	0	0	2
5	0	0	0	1	0	1	0	0	0	0	0	0	2
6	1	0	0	0	1	0	0	0	0	0	0	0	2
7	0	0	0	0	0	0	0	1	0	0	0	1	2
8	0	0	0	0	0	0	1	0	1	0	0	0	2
9	0	0	0	0	0	0	0	1	0	1	0	0	2
10	0	0	0	0	0	0	0	0	1	0	1	0	2
11	0	1	0	0	0	0	0	0	0	1	0	3	5
12	1	0	0	0	0	0	1	0	0	0	3	0	5
CS	5	5	2	2	2	2	2	2	2	2	5	5	36

Figure 1. Diphenylene DPH and its numbering.

In graphs containing rings, more than one path could join the pair (i,j), resulting in more than one fragment related to i (with respect to j and a given path p). The entries in the Cluj matrix are taken, by definition, as the maximum cardinality among all such fragments:

$$[UCJ]_{i,j} = \max_p |CJ_{i,j,p}| \qquad (4)$$

In trees, due to the unique nature of paths joining any two vertices, $CJ_{i,j,p}$ represents the set of paths going to j through i. In this way, the path $p(i,j)$ is characterized by a single endpoint, which is sufficient for the unsymmetric matrix **UCJ**. When the path p belongs to the set of distances $DI(G)$, the suffix DI is added to the name of matrix, as in **UCJDI**. When path p belongs to the set of detours $DE(G)$, the suffix is DE. The Cluj matrices are defined in any graph and, except for some symmetric graphs, are unsymmetric and can be symmetrized by the Hadamard multiplication with their transposes

$$SM_p = UM \bullet (UM)^T \qquad (5)$$

If the matrices calculated from edges (i.e., on adjacent vertex pairs) are required, the matrices calculated from paths must be multiplied by the adjacency matrix **A** (which has the nondiagonal entries of 1 if the vertices are joined by an edge and, otherwise, zero)

$$SM_e = SM_p \bullet A \qquad (6)$$

The basic properties and applications of the above matrices and derived descriptors have been presented elsewhere.[31−34] Examples of Cluj matrices, calculated on distance or detour, are given in Chart 1; the numbering is shown in Figure 1.

3. CLUJ POLYNOMIALS

The Cluj polynomials are defined on the basis of Cluj matrices as

$$CJ(G,x) = \sum_k m(G,k)x^k \qquad (7)$$

They count the vertex proximity of the vertex i with respect to any vertex j in G, joined to i by an edge $\{p_{e,i}\}$ (the Cluj-edge polynomials) or by a path $\{p_{p,i}\}$ (the Cluj-path polynomials), taken as the shortest (distance DI) or the longest (detour DE) paths. In eq 7, the coefficients $m(G,k)$ are calculated from the entries of Cluj matrices. The summation runs up to the maximum $k = |\{p\}|$ in G.

2. CLUJ MATRICES

A Cluj fragment,[1,31−34] $CJ_{i,j,p}$, collects vertices v lying closer to i than to j, the endpoints of a path $p(i,j)$. Such a fragment collects the vertex proximity of i against any vertex j, joined by the path p, with the distances measured in the subgraph $D_{(G-p)}$, as shown in the following equation:

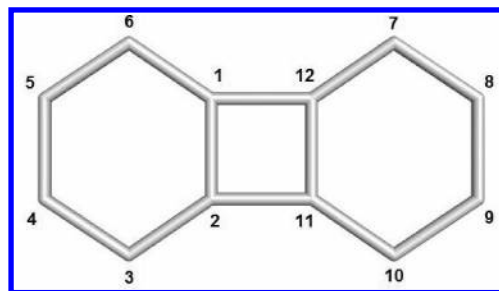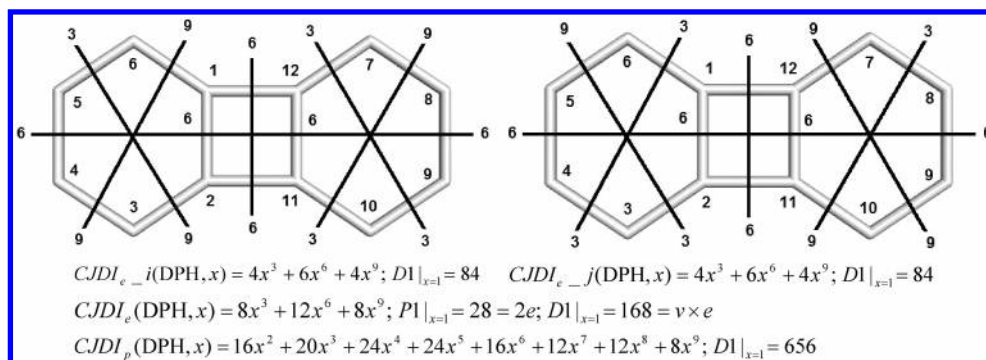$$CJ_{i,j,p} = \{v | v \in V(G); D_{(G-p)}(i,v) < D_{(G-p)}(j,v)\} \quad (3)$$

$CJDI_{e\_i}(DPH,x) = 4x^3 + 6x^6 + 4x^9; D1|_{x=1} = 84$ $CJDI_{e\_j}(DPH,x) = 4x^3 + 6x^6 + 4x^9; D1|_{x=1} = 84$

$CJDI_e(DPH,x) = 8x^3 + 12x^6 + 8x^9; P1|_{x=1} = 28 = 2e; D1|_{x=1} = 168 = v \times e$

$CJDI_p(DPH,x) = 16x^2 + 20x^3 + 24x^4 + 24x^5 + 16x^6 + 12x^7 + 12x^8 + 8x^9; D1|_{x=1} = 656$

Figure 2. Edge cut procedure for calculating Cluj polynomial $CJDI_e$ in diphenylene DPH.

Table 1. Cluj $CJDI_e$ and Related Polynomials in Phenylenes PHE_h; h = Number of Hexagons in Molecule

$$CJDI_e(PHE_h,x) = 4\sum_{k=1}^{h-1} x^{6k} + 8\sum_{k=0}^{h-1} x^{6k+3} + 4hx^{3h}; D1|_{x=1} = 48h^2 - 12h = 6h(8h - 2) = ve$$

$$\Omega(PHE_h,x) = (3h - 1)x^2 + x^{2h}; D1|_{x=1} = e = 8h - 2$$

$$CI(PHE_h) = 4(3h - 1)(5h - 2)$$

$$\Omega(PHE_h, x)|_{x=1} = 3h = v/2$$

$$N\Omega(PHE_h,x) = 2hx^{(6h-2)} + 2(3h - 1)x^{4(2h-1)}; D1|_{x=1} = 4(3h - 1)(5h - 2)$$

Table 2. Cluj $CJDI_e$ and Related Polynomials in Spiranes SP_h; h = Number of Hexagons in Molecule

$$CJDI_e(SP_{1,3},x) = (8 + 2h)x^3 + 8\sum_{k=2}^{h-1} x^{(5k-2)} + (8 + 2h)x^{5h-2}; D1|_{x=1} = ev$$

$$CJDI_e(SP_{1,4},x) = 12 \sum_{k=1}^{h} x^{(5k-2)}; D1|_{x=1} = ev$$

$$CJDI_e(SP_{1,3;1,4},x); D1|_{x=1} = ev = 6h(5h + 1)$$

$$\Omega(SP_{1,3;1,4},x) = 3hx^2; D1|_{x=1} = e = 6h \text{ and } v = 5h + 1$$

$$N\Omega(SP_{1,3;1,4},x) = 6hx^{(e-2)} = 6hx^{(6h-2)}; D1|_{x=1} = 12h(3h - 1)$$

Table 3. Cluj $CJDI_e$ and Related Polynomials in Pyrenes $PYR_{p/h}$ (d-Condensed Pyrenes, See #10, Table 14); p = PYR Units; h = Number of Hexagons in Molecule

$$CJDI_e(PYR_p,x) = 4px^3 + 12\sum_{k=0}^{p-1} x^{(5+14k)} + 2(2p + 1)x^{7p+1} + 12\sum_{k=0}^{p-1} x^{(11+14k)} + 4px^{14p-1}; D1|_{x=1} = ev$$

$$ev = 2(18p + 1)(7p + 1) = D1[CJDI_e(PYR_p,x)]|_{x=1}$$

$$\Omega(PYR_p,x) = 2px^2 + 4px^3 + x^{2p+1}; D1|_{x=1} = e = 18p + 1; v = 2(7p + 1)$$

$$N\Omega(PYR_p,x) = 4px^{(18p-1)} + 12px^{(18p-2)} + (2p + 1)x^{16p}; D1|_{x=1} = 4p(80p - 3)$$

$$CJDI_e(PYR_h,x) = hx^3 + 12\sum_{k=0}^{h/4-1} x^{(5+14k)} + (h + 2)x^{7h/4+1} + 12\sum_{k=0}^{h/4-1} x^{(11+14k)} + hx^{7h/2-1}; D1|_{x=1} = ev$$

$$ev = (9h/2 + 1)(7h/2 + 2) = D1[CJDI_e(PYR_h,x)]|_{x=1}$$

$$\Omega(PYR_h,x) = h/2x^2 + hx^3 + x^{h/2+1}; D1|_{x=1} = e = 9h/2 + 1; v = 7h/2 + 2$$

$$N\Omega(PYR_h,x) = hx^{(9h/2-1)} + 3hx^{(9h/2-2)} + (h/2 + 1)x^{4h}; D1|_{x=1} = h(20h - 3)$$

The Cluj polynomials published previously[26] referred to some partitions of the Cluj matrices given by the layer/shell matrices and provide no direct interpretation of the counting content.

The polynomial coefficients are counted from the Cluj matrices by the TOPOCLUJ software program[30] and also by a simple routine for collecting the entries in the unsymmetric matrices **UCJ**. In the case of the $CJDI_e$ polynomial, an orthogonal edge-cutting procedure can be used, as shown in Figure 2. The same procedure has been used by Gutman

and Klavžar to calculate the Szeged index of polyhex graphs.[35]

In this paper, $v = v(G) = |V(G)|$ and $e = e(G) = |E(G)|$ refer to the cardinality of the vertex and edge sets, respectively.

Since the Cluj matrices are unsymmetric, two polynomials can be written, one with respect to the endpoint i (and to the first triangle of the **UCJDI**$_e$ matrix) and the other one referring to the endpoint j of the edge $e(i,j)$ (and to the second triangle of that matrix). They depend, however, on the

Table 4. Cluj $CJDI_e$ and Related Polynomials in Coronenes CORr; r = Number of Hexagon Rows around the Central Hexagon

$$CJDI_e(COR_r,x) = \sum_{k=0}^{r} 6(r + k + 2)x^{(k+1)(2r+k+3)} + \sum_{k=0}^{r-1} 6(r + k + 2)x^{6(r+1)^2-(k+1)(2r+k+3)}; D1|_{x=1} = ev$$

$$ev = 18(r + 1)^3(3r + 2) = D1[CJDI_e(COR_r,x)]|_{x=1};$$

$$ev = 18(r)^3(3r - 1) = D1[CJDI_e(COR_r,x)]|_{x=1}$$

$$v = 6(r + 1)^2; f = 3r(r + 1) + 2; e = 3(r + 1)(3r + 2)$$

$$\Omega(COR_r,x) = 6\sum_{k=2}^{(r+1)} x^{(r+k)} + 3x^{2(r+1)}; D1|_{x=1} = 3(r + 1)(3r + 2) = e$$

$$N\Omega(COR_r,x) = \sum_{k=2}^{r+1} 6(r + k)x^{[e-(r+k)]} + 6(r + 1)x^{[e-2(r+1)]}; D1|_{x=1} = (r + 1)(81r^3 + 175r^2 + 119r + 24)$$

numbering, and only their sum polynomial is an invariant (see Figure 2). Only this last polynomial will be considered in the following discussion.

4. PROPERTIES OF THE CLUJ AND RELATED POLYNOMIALS

Among the properties of counting polynomials, the value in $x = 1$ and the first derivative in $x = 1$ are the most important. In the case of the $CJDI_e$ polynomial, the value in $x = 1$ is $P|_{x=1} = 2e$. It is evident, since every edge is visited twice. The first derivative, in $x = 1$, gives the meaning of the topological property collected by a matrix or a polynomial. In this case, the following theorem holds:

Theorem 1. *In a bipartite graph, the sum of all edge-counted vertex proximities equals the product $v \times e$ of the number of vertices and edges in G.*

Demonstration. In a bipartite, planar graph, in which orthogonal edge cuts are permitted, for every edge $e(i,j) \in E(G)$, there is a clear separation of vertex proximities $\{p_{e,i}\}$ and $\{p_{e,j}\}$ of its endpoints. If we denote the cardinalities of the above sets by $p_{e,i}$ and $p_{e,j}$, then in a bipartite graph

$$p_{e,i} + p_{e,j} = v \qquad (8)$$

It follows that, for all edges, $e \in E(G)$, the total of edge-counted vertex proximities p_e equals the product $v \times e$, thus demonstrating the theorem.

An orthogonal or an elementary edge cut of a (polycyclic) bipartite planar graph G is a straight line segment, orthogonal to and passing through the centers of some edges of the graph, intersecting the perimeter of G exactly two times, so that at least one polygon lies between these two intersection points.[1,35] Trees also allow elementary edge cuts.

In the orthogonal edge-cut procedure used to calculate the $CJDI_e$ index (i.e., the half-sum of all entries in the matrix **CJDI$_e$**), the total of edge-counted vertex proximities $p_e = CJDI_e(G,x); D1|_{x=1}$ is calculated as

$$p_e = \sum_c m(G,c) \, c(p_{e,i} + p_{e,j}) = v\sum_c m(G,c) \, c = v \times e \qquad (9)$$

where the coefficients $m(G,c)$ are related to the occurrence of edge cuts of extent c and $\sum_c m(G,c) \, c = e(G)$. The above theorem can be extended to 3D bipartite molecular structures, although the separation of the proximities is less obvious in this case. Numerical results provided by the Cluj matrix support this extension.

Corollary to Theorem 1. *In bipartite graphs, there are no equidistant vertices with respect to the two endpoints of any edge.*

The Cluj matrix counts the vertices lying closer to each of the endpoints of any edge and leaves the equidistant vertices uncounted. Because of relation 8, it follows that, in bipartite graphs, all vertices are counted and *no equidistant vertices* exist. Next, for all of the edges in G, one obtains the total of vertex proximities, p_e, equal to $v \times e$. This is the main result provided by the Cluj matrix/polynomial. The vertex proximity calculation could be of interest in calculating the *bond polarity* and molecular dipole moments. In this respect, weighted molecular graphs must be used.

It may be recalled that equidistant vertices are also not counted in calculating the Szeged index,[35-38] a topological index related to the Wiener index,[39] which counts all the shortest distances in a graph.

Theorem 2. *In a tree graph G, the sum of all path-counted vertex proximities is twice the sum of all distances in G or twice the Wiener index W: $p_p = CJDI_p(G,x); D1|_{x=1} = 2W$.*

Demonstration. The column sums in the **UCJDI$_p$** matrix equal the column sums in the matrix of distances, while the row sums in the **UCJDI$_p$** matrix are identical to those in the Wiener matrix.[1] It is known that the half sum of entries in these matrices counts all the distances in a tree graph, or the Wiener index. Since the first derivative of the $CJDI_p$ polynomial is the sum of all entries in **UCJDI$_p$**, it follows that $p_p = CJDI_p(G,x); D1|_{x=1} = 2W$, thus demonstrating the theorem.

In graphs containing rings, the Cluj index $CJDI_p$ however is different from both the Wiener and Szeged indices.[1] Formulas for calculating the Cluj $CJDI_e$ and related polynomials (see below), in phenylenes, spiranes, pyrenes, and coronenes, are given in Tables 1−4.
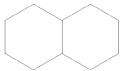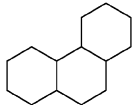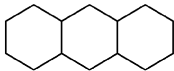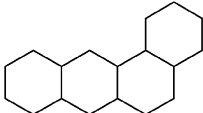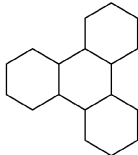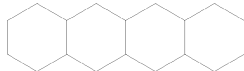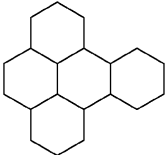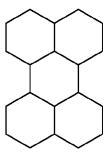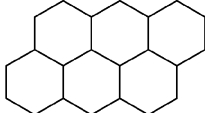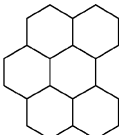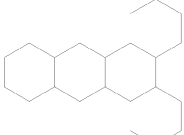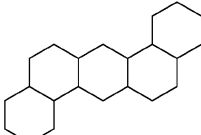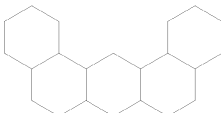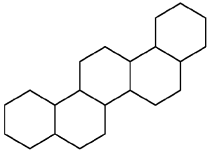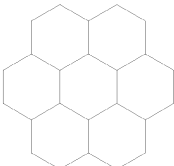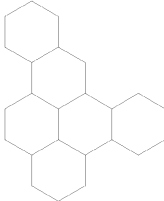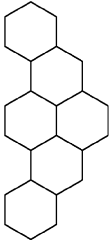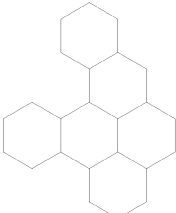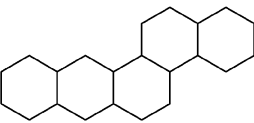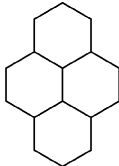
Two related polynomials are included in the above tables. One is the Omega polynomial, $\Omega(G,x)$, proposed by Diudea[40] for counting the orthogonal edge cuts, and the second one is the "non-Omega" $N\Omega(G,x)$ polynomial, which is somewhat complementary to the Omega polynomial. It has been shown[40,41] that the edges forming an edge-cut strip are locally codistant, or equidistant and "topologically" parallel.

Let $m(G,c)$ denote the occurrence of the edge cut of length c (i.e., the number of edges cut off) in G. In a bipartite, planar graph, the two polynomials are defined as

$$\Omega(G,x) = \sum_c m(G,c) \, x^c \qquad (10)$$

$$N\Omega(G,x) = \sum_c m(G,c) \, cx^{(e-c)} \qquad (11)$$

Table 5. Polyhex Molecules Tested for Correlation vs BP and I_{chr} with $\Omega(G,x)$ as an Identifier

1 $3x^2$	**2** $4x^2 + x^3$	**3** $5x^2 + 2x^3$	**4** $6x^2 + x^4$
5 $6x^2 + 3x^3$	**6** $7x^2 + x^3 + x^4$	**7** $6x^2 + 3x^3$	**8** $8x^2 + x^5$
9 $4x^2 + 4x^3 + x^4$	**10** $4x^2 + 4x^3 + x^4$	**11** $5x^2 + 2x^3 + 2x^4$	**12** $2x^5 + 5x^3 + 2x^4$
13 $2x^2 + 5x^3 + 2x^4$	**14** $8x^2 + 2x^3 + x^4$	**15** $8x^2 + 2x^3 + x^4$	**16** $8x^2 + 2x^3 + x^4$
17 $7x^2 + 4x^3$	**18** $6x^3 + 3x^4$	**19** $6x^2 + 3x^3 + 2x^4$	**20** $6x^2 + 3x^3 + 2x^4$
21 $6x^2 + 3x^3 + 2x^4$	**22** $6x^2 + 3x^3 + 2x^4$	**23** $8x^2 + 2x^3 + x^4$	**24** $2x^2 + 5x^3$

Their $D1|_{x=1}$'s give the total number of equidistant and non-equidistant edges versus each edge in G

$$\Omega(G,x)D1|_{x=1} = e = |E(G)| \qquad (12)$$

$$N\Omega(G,x)D1|_{x=1} = PI(G) \qquad (13)$$

where $PI(G)$ is Khadikar's topological index.[42]

Two indices have been defined on the basis of the Omega polynomial. The first, CI, is derived from the first and second derivatives, in $x = 1$, as

$$CI(G) = [\Omega(G,x)D1]^2 - $$
$$[\Omega(G,x)D1 + \Omega(G,x)D2]|_{x=1} \qquad (14)$$

The second descriptor can be calculated from all possible

CLUJ AND RELATED POLYNOMIALS

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Table 6. Properties and Topological Indices of the Molecular Structures from Table 5

G	BP	I_{CHR}	$UCJDI_p$	$UCJDE_p$	I_Ω	CI	$SCJDI_p$	$SCJDE_p$	$SCJDI_e$	$SCJDE_e$
1	80.1		72	36	1.408	24	90	24	54	6
2	218	1784	362	142	1.505	96	663	129	243	19
3	338	2874	1050	322	1.436	218	2547	326	632	32
4	340	2800	1044	340	1.624	216	2584	402	656	32
5	431	4198	2303	608	1.385	390	7133	701	1325	71
6	425	4169	2308	592	1.522	388	7125	646	1301	85
7	429	4017	2352	654	1.385	390	7110	753	1269	45
8	440		2298	614	1.754	384	7269	733	1381	61
9	496	5488	3246	750	1.520	508	11 475	778	1887	56
10	493	4650	3306	744	1.520	508	11 906	752	1852	66
11	497	4739	3326	742	1.555	506	12 581	801	1858	56
12	547	5439	4382	894	1.538	644	17 473	893	2613	56
13	542	5262	4452	884	1.538	644	18 272	917	2571	67
14	535	5099	4392	1044	1.455	610	16 309	1296	2290	74
15	536	5325	4318	1000	1.455	610	16 336	1357	2354	82
16	531		4290	996	1.455	610	15 927	1325	2290	82
17	519		4324	952	1.348	612	16 377	1136	2330	82
18	590	5821	5814	1080	1.539	798	26 469	1125	3438	66
19	592		5821	1142	1.484	758	24 395	1265	3095	78
20	596		5710	1100	1.484	758	23 723	1191	3174	69
21	594		5793	1153	1.484	758	24 036	1312	3023	78
22	595		4301	973	1.506	756	16 256	1206	2354	86
23		5488	5722	1104	1.455	610	23 763	1211	3174	68
24		3301	1618	464	1.470	308	4719	443	1008	43

Table 7. Correlating Ability of Descriptors from Table 6 in Mono and Bivariate Regression against BP

	monovariate			bivariate		
	indices	R	CV%	indices	R	CV%
1	$UCJDE_p$	0.963 09	7.66	$SCJDI_p$, CI	**0.991**	**3.7894**
2	CI	0.964	7.51	$UCJDI_p$, CI	**0.987 37**	**4.62**
3	$SCJDI_e$	0.935	10.053	$SCJDI_e$, CI	**0.9864**	**4.791**
4	$UCJDI_p$	0.934	10.165	$SCJDE_e$, CI	0.9728	6.756
5	$SCJDE_p$	0.915	11.477	$UCJDE_p$, CI	0.967	7.401
6	$SCJDI_p$	0.8943	12.738	$SCJDE_p$, CI	0.965	7.559
7	$SCJDE_e$	0.8466	15.171			
8	I_Ω	0.0573	28.247			

Table 8. Correlating Ability of Descriptors from Table 6 in Mono- and Bivariate Regression against I_{chr}

	monovariate			bivariate		
	indices	R	CV%	indices	R	CV%
1	CI	0.964	7.371	$SCJDI_p$, CI	**0.985**	**4.937**
2	$UCJDE_p$	0.957	8.045	$SCJDI_e$, CI	0.978	5.958
3	$UCJDI_p$	0.948	8.77	$UCJDI_p$, CI	0.974	6.442
4	$SCJDI_e$	0.940	9.432	$SCJDE_e$, CI	0.970	6.88
5	$SCJDI_p$	0.907	11.633	$UCJDE_p$, CI	0.967	7.336
6	$SCJDE_p$	0.8822	13.069	$SCJDE_p$, CI	0.965	7.491
7	$SCJDE_e$	0.780	17.36			

derivatives Dn, in $x = 1$, and normalized to the first derivative (which equals the number of edges in G)

$$I_\Omega(G) = [1/\Omega(G,x)D1]\sum_n [\Omega(G,x)Dn]^{1/n}|_{x=1} \quad (15)$$

Theorem 3. *In a bipartite planar graph, CI and PI indices are identical.*

Demonstration. From eqs 11 and 13, writing $m(G,c)$ simply as m, the *PI* index can be calculated as

$$PI(G) = \sum_c mc(e - c) = e\sum_c mc -$$
$$\sum_c mc^2 = e^2 - \sum_c mc^2 \quad (16)$$

CI may always be calculated using the relation developed by the expansion of eq 14 as

$$CI(G) = \sum_c (mc)^2 - \sum_c [mc + mc(c - 1)] =$$
$$\sum_c = e^2 - \sum_c mc^2 = PI(G) \quad (17)$$

In the above, the following relation holds:

$$e(G) = \sum_c mc = \Omega(G,x)D1|_{x=1} = N\Omega(G,x)|_{x=1} \quad (18)$$

However, eq 11 is not always valid, so that *CI* is, in general, different from *PI*, except in the case of bipartite planar graphs. Equation 16 was proposed by John et al.[43] for computing *PI* in benzenoid hydrocarbon graphs.

In bipartite graphs which can be embedded in surfaces of $g > 0$, for example, in toroidal polyhexes, relation 11 is more obscure, notwithstanding $CI = PI$. In the case of the torus T(6,3)H:[8,12] $\Omega(G,x) = 12x^4 + 4x^{24}$, $e = 144$, $CI = 18\,240$, $N\Omega(G,x) = 96x^{122} + 48x^{136}$, and $PI = 18\,240$. According to eq 11, the polynomial would be $N\Omega(G,x) = 96x^{120} + 48x^{140}$; this gives the same *PI* index value. Currently, no generalization of this case could be found.

The $CJDI(G,x)$ and $N\Omega(G,x)$ polynomials describe, in the same manner, collections of nonequidistant subgraphs (vertices and edges, respectively), addition being the most simple and natural operation. Applications of these descriptors are described below.

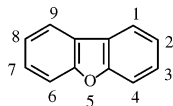## 5. CORRELATING ABILITY OF CLUJ AND RELATED DESCRIPTORS

To test the correlating ability of Cluj descriptors, we selected different types of planar polyhex structures, dibenzofurans, coronenes, and pyrenes.

5.1. Boiling Point and Chromatographic Retention Index of Polyhexes. The physicochemical properties estimated for the structures in Table 5 are the boiling

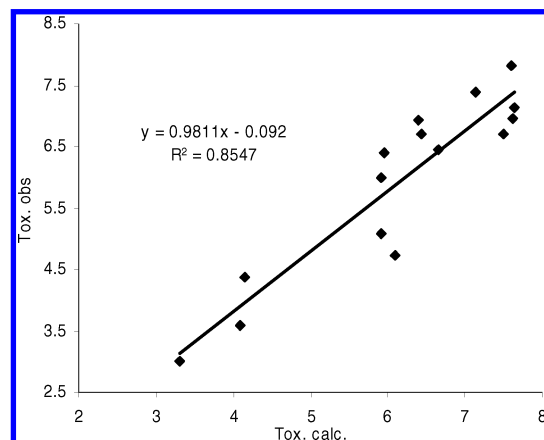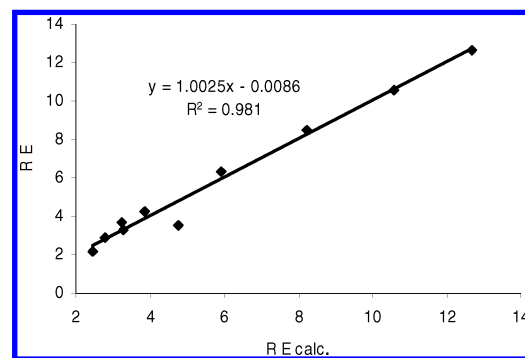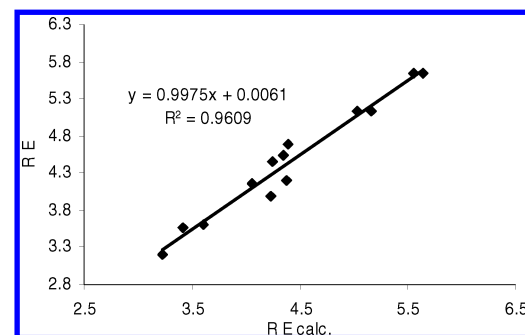**Table 9.** Intercorrelating Matrix of the Descriptors from Table 6

	CI	I_Ω	$SCJDE_e$	$UCJDE_p$	$SCJDE_p$	$SCJDI_e$	$UCJDI_p$	$SCJDI_p$
CI	1	0.019	0.788	**0.984**	0.922	**0.993**	**0.993**	**0.976**
I_Ω		1	0.124	0.066	0.114	0.002	0.088	0.036
$SCJDE_e$			1	0.838	0.865	0.733	0.755	0.685
$UCJDE_p$				1	**0.973**	0.965	**0.978**	0.945
$SCJDE_p$					1	0.893	0.919	0.873
$SCJDI_e$						1	**0.995**	**0.992**
$UCJDI_p$							1	**0.991**
$SCJDI_p$								1

Table 10. Structure and AhR Binding Affinity Data for Chlorinated Dibenzofurans

structure	substituent	toxicity (pEC_{50})
	9 1	
	8 2	
	7 3	
	6 5 4 O	
1	2-Cl	3.553
2	3-Cl	4.377
3	4-Cl	3.000
4	2,3-diCl	5.326
5	2,6-diCl	3.609
6	2,8-diCl	3.590
7	1,2,7-trCl	6.347
8	1,3,6-trCl	5.357
9	1,3,8-trCl	4.071
10	2,3,4-trCl	4.721
11	2,3,8-trCl	6.000
12	1,2,3,6-teCl	6.456
13	1,2,3,7-teCl	6.959
14	1,2,4,8-teCl	5.000
15	2,3,4,6-teCl	6.456
16	2,3,4,7-teCl	7.602
17	2,3,4,8-teCl	6.699
18	2,3,6,8-teCl	6.658
19	2,3,7,8-teCl	7.387
20	1,2,3,4,8-peCl	6.921
21	1,2,3,7,8-peCl	7.128
22	1,2,3,7,9-peCl	6.398
23	1,2,4,6,7-peCl	7.169
24	1,2,4,6,8-peCl	5.509
25	1,2,4,7,8-peCl	5.886
26	1,2,4,7,9-peCl	4.699
27	1,3,4,7,8-peCl	6.699
28	2,3,4,7,8-peCl	7.824
29	2,3,4,7,9-peCl	6.699
30	1,2,3,4,7,8-heCl	5.081
31	1,2,3,6,7,8-heCl	3.000
32	1,2,4,6,7,8-heCl	3.553
33	2,3,4,6,7,8-heCl	4.377
34	dibenzofuran	3.000

Figure 3. Dibenzofurans; predicted vs observed toxicity.

$y = 0.9811x - 0.092$
$R^2 = 0.8547$

Figure 4. Plot of resonance energy against that calculated by Cluj descriptors (Table 16).

$y = 1.0025x - 0.0086$
$R^2 = 0.981$

Figure 5. Plot of resonance energy against that calculated by eq 21.

$y = 0.9975x + 0.0061$
$R^2 = 0.9609$

point (BP) and chromatographic retention index (I_{chr}).[44,45] The goal of this study was not to find the best model for a given molecular property but to obtain information about the possibility of using the Cluj and related descriptors in correlating studies. Accordingly, only mono- and bivariate regressions were considered. Table 5 also includes $\Omega(G,x)$ as an identifier of the planar polyhex structures.

The properties and topological indices of the set of structures in Table 5 are listed in Table 6. Statistics of the test are listed in Tables 7 and 8. Both indices derived from the Omega polynomial show the same degeneracy. It is as expected, since both indices are calculated on this polynomial, which is also degenerate, exactly on the same structures.

Also as expected, the indices belonging to the same class are highly intercorrelated (here, in bold, with the threshold 0.97). The high correlation of *CI* with the Cluj descriptors is quite surprising. By contrast, I_Ω is practically orthogonal to all of these descriptors (Table 9).

In monovariate regression, we can consider a good correlation to be one with CV% < 10. In the case of BP, all but I_Ω show a significant correlation. However, only that of

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Table 11. Partial Charges (Ch), Regression Coefficients (c_i), and Ct_{DBF} in Dibenzofurans

molecule	Ch_2	Ch_3	Ch_4	Ch_5	Ch_7	Ch_9	Ch_{10}	Ch_{11}	Ch_{13}	$Ct_{DBF}{}^a$
c_i	−19.930	59.797	−59.850	80.2617	183.342	50.880	−44.714	−3.618	−12.829	29.5917[b]
1	−0.039	−0.127	−0.073	−0.108	−0.079	−0.096	−0.079	−0.149	−0.045	3.814
2	−0.041	−0.126	−0.074	−0.107	−0.078	−0.112	−0.101	−0.130	−0.030	4.152
3	−0.040	−0.127	−0.074	−0.106	−0.069	−0.141	−0.081	−0.115	−0.045	3.460
4	−0.038	−0.126	−0.072	−0.107	−0.077	−0.101	−0.113	−0.161	−0.034	5.403
5	−0.042	−0.114	−0.079	−0.141	−0.067	−0.093	−0.077	−0.149	−0.043	4.525
6	−0.042	−0.150	−0.077	−0.095	−0.077	−0.095	−0.077	−0.150	−0.042	4.117
7	−0.028	−0.127	−0.099	−0.111	−0.075	−0.096	−0.067	−0.161	−0.083	5.614
8	−0.044	−0.111	−0.078	−0.140	−0.065	−0.112	−0.091	−0.135	−0.061	4.999
9	−0.045	−0.147	−0.076	−0.093	−0.075	−0.114	−0.091	−0.136	−0.061	4.630
10	−0.037	−0.125	−0.071	−0.105	−0.067	−0.143	−0.128	−0.150	−0.038	5.954
11	−0.041	−0.149	−0.076	−0.093	−0.075	−0.100	−0.112	−0.161	−0.031	5.708
12	−0.043	−0.110	−0.076	−0.141	−0.064	−0.102	−0.103	−0.174	−0.073	6.479
13	−0.027	−0.126	−0.099	−0.110	−0.073	−0.102	−0.104	−0.174	−0.074	7.305
14	−0.042	−0.147	−0.074	−0.092	−0.064	−0.135	−0.073	−0.151	−0.088	5.064
15	−0.040	−0.112	−0.076	−0.140	−0.055	−0.142	−0.128	−0.150	−0.036	6.425
16	−0.025	−0.128	−0.099	−0.109	−0.064	−0.142	−0.128	−0.150	−0.037	7.359
17	−0.040	−0.149	−0.074	−0.091	−0.064	−0.143	−0.127	−0.151	−0.035	6.192
18	−0.045	−0.138	−0.083	−0.130	−0.063	−0.098	−0.111	−0.162	−0.029	6.084
19	−0.030	−0.161	−0.112	−0.099	−0.073	−0.099	−0.112	−0.161	−0.030	6.880
20	−0.043	−0.147	−0.075	−0.093	−0.073	−0.104	−0.103	−0.175	−0.073	6.149
21	−0.032	−0.159	−0.112	−0.099	−0.072	−0.102	−0.103	−0.174	−0.073	7.321
22	−0.060	−0.140	−0.089	−0.116	−0.073	−0.105	−0.102	−0.178	−0.073	5.764
23	−0.030	−0.115	−0.113	−0.152	−0.053	−0.134	−0.073	−0.150	−0.089	6.288
24	−0.045	−0.137	−0.082	−0.130	−0.053	−0.135	−0.072	−0.151	−0.087	5.213
25	−0.031	−0.159	−0.111	−0.098	−0.062	−0.135	−0.072	−0.151	−0.088	6.163
26	−0.058	−0.140	−0.088	−0.116	−0.064	−0.137	−0.071	−0.155	−0.088	4.551
27	−0.032	−0.158	−0.112	−0.097	−0.063	−0.157	−0.104	−0.123	−0.066	6.204
28	−0.029	−0.161	−0.111	−0.097	−0.063	−0.143	−0.127	−0.150	−0.034	7.294
29	−0.060	−0.134	−0.090	−0.112	−0.063	−0.142	−0.127	−0.148	−0.038	7.185
30	−0.031	−0.159	−0.111	−0.097	−0.061	−0.148	−0.117	−0.164	−0.078	7.667
31	−0.036	−0.148	−0.127	−0.143	−0.061	−0.101	−0.102	−0.174	−0.072	7.349
32	−0.036	−0.148	−0.126	−0.143	−0.063	−0.094	−0.063	−0.162	−0.081	5.686
33	−0.033	−0.150	−0.127	−0.142	−0.053	−0.142	−0.127	−0.150	−0.033	7.184
34	−0.042	−0.128	−0.076	−0.109	−0.081	−0.109	−0.076	−0.128	−0.042	2.534

[a] Global descriptor of partial charges in DBF set. [b] Intercept term.

Table 12. Data for the Training Set of Dibenzofurans

molecule	Ct_{DBF}	$C_{(LM\_W\_CJDI_e\_SGI)}$	toxicity units
1	3.814	0.971	3.553
4	5.403	0.916	5.326
5	4.525	0.974	3.609
7	5.614	1.3	6.347
8	4.999	0.97	5.357
9	4.630	1.162	4.071
14	5.064	0.953	5
15	6.425	0.943	6.456
16	7.359	1.095	7.602
17	6.192	1.165	6.699
18	6.084	1.16	6.658
23	6.288	1.205	7.169
24	5.213	0.962	5.509
25	6.163	1.191	5.886
26	4.551	1.22	4.699
34	2.534	0.729	3

Table 13. Data for the Testing Set of Dibenzofurans

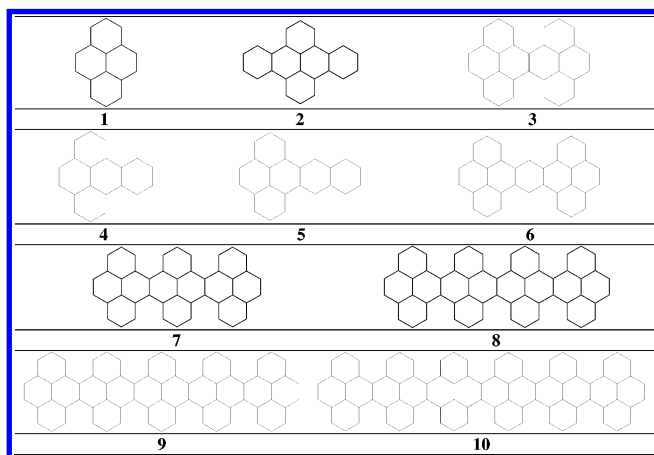| molecule	Ct_{DBF}	$C_{(LM\_W\_CJDI_e\_SGI)}$	toxicity (pEC$_{50}$)	toxicity (pEC$_{50}$) calcd
2	4.152	0.94	4.377	4.140
3	3.460	0.723	3	3.299
6	4.117	0.916	3.59	4.091
10	5.954	0.942	4.721	6.087
11	5.708	1.134	6	5.903
12	6.479	0.946	6.456	6.656
13	7.305	1.097	6.959	7.613
19	6.880	1.07	7.387	7.142
20	6.149	1.18	6.921	6.399
21	7.321	1.103	7.128	7.632
22	5.764	1.128	6.398	5.961
27	6.204	1.123	6.699	6.435
28	7.294	1.1	7.824	7.602
29	7.185	1.126	6.699	7.496
32	5.686	1.194	5.081	5.905

$UCJDE_p$ and CI is acceptable. In the case of I_{chr}, four descriptors exceeded the percent of covariance (CV%) threshold of 10.

In bivariate regression, the threshold for good correlation was taken as CV% < 5. In the case of BP, three pairs of descriptors fulfilled this condition, while in the case of I_{chr}, only one pair of descriptors succeeded in surpassing the threshold. This ensures a Pearson correlation coefficient R > 0.97, a threshold also providing a good correlation. In all the bivariate correlations, CI is the pair; no pair of exclusively Cluj descriptors could provide a good correlation. This

demonstrates that CI, along with the Cluj descriptors, is a good descriptor in correlating studies. The CV% and the Pearson coefficient R are good indicators of the quality of the regression equation.

No linear size effect was inferred from the above study, but a clear structure−property correlation is manifested. Our results are at least as good as those reported earlier by Randić.[44,45]

Table 9 shows an intercorrelating matrix of the descriptors from Table 6.

Table 14. Molecular Structures of Pyrenes

Table 16. Data for the Pyrenes from Table 14

structure	UCJDI$_p$	SCJDI$_e$	RE (eV)	RE calcd
1	1618	1008	2.133	2.446
2	5846	3096	3.669	3.220
3	11854	5781	4.243	3.874
4	3306	1852	2.906	2.771
5	5826	3128	3.319	3.283
6	17318	8410	3.527	4.765
7	38812	17260	6.351	5.905
8	90761	38385	8.459	8.240
9	175950	72096	10.571	10.592
10	302590	121333	12.675	12.698

was generated and correlated on an ad hoc basis with the property studied. Partial charges, calculated with the PM3 Hamiltonian,[51] and the coefficients of autocorrelation[52,53] are listed in Table 11. The last column contains the global descriptor Ct$_{DBF}$, which is a linear combination of the local partial charges fitted to the autocorrelation equation. We associated this global descriptor with an index of centrality,[1] $C_{(LM\_W\_CJDI_e\_SGI)}$ calculated on the Cluj matrix **CJDI$_e$** with a weighting scheme using Sanderson group electronegativities, SGI,[28] to account for the chemical nature of atoms in molecules. A subset of 16 dibenzofurans (Table 12) was randomly selected as the training set, and in a "leave-half-out" approach, 15 structures (Table 13) were used as the
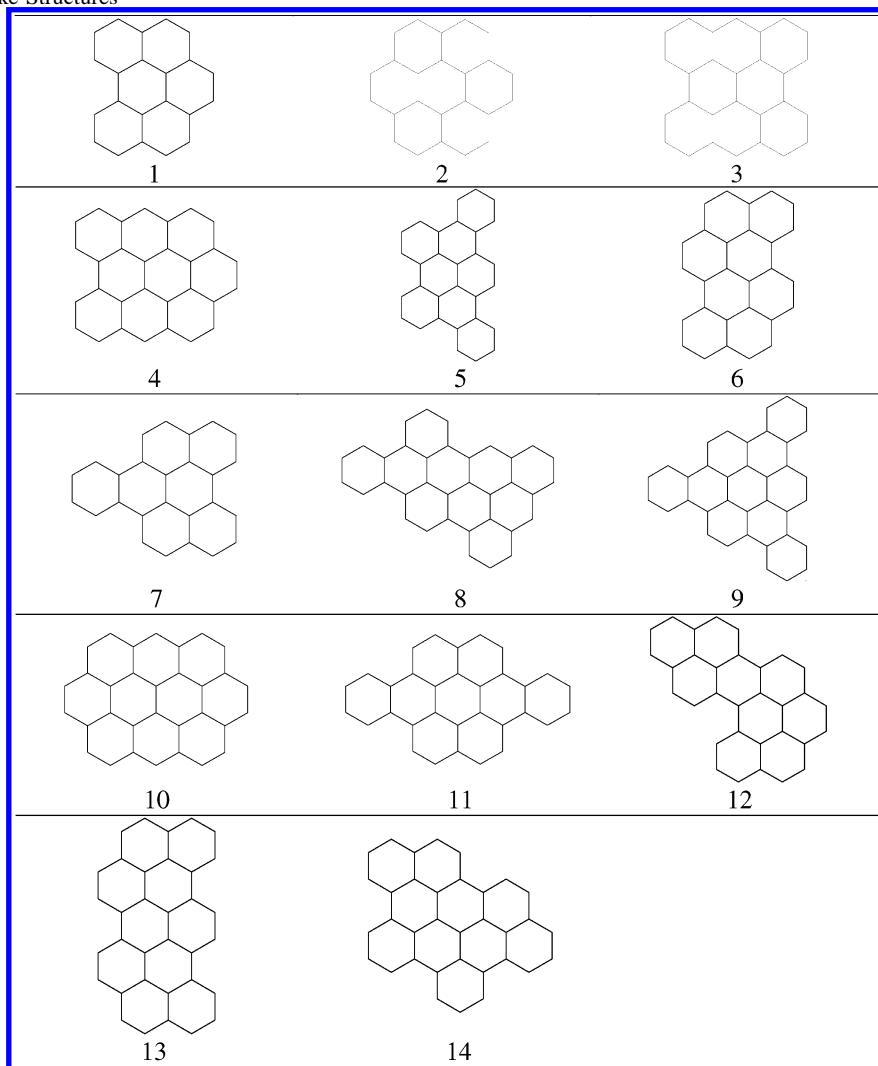
5.2. Toxicity of Dibenzofurans. Dibenzofurans are industrially important and are known for their wide distribution, resistance to biological and chemical degradations, high toxicity, and bioaccumulation.[46,47] Some of them cause toxic effects after binding to an intracellular cytosolic receptor, the aryl hydrocarbon receptor (AhR).[48,49]

To describe the structure of dibenzofurans[50] in Table 10, a very simple electronic descriptor based on partial charges

Table 15. Coronene-Like Structures

Table 17. Data for the Set of Coronenes from Table 16

structure	I	HOMO (eV)	UCJDip	RE (eV)	RE_{calcd} (eV)	residual
1	1.538	−9.513	4452	3.15	3.1187	0.0313
2	1.539	−9.280	5814	3.509	3.31629	0.192 71
3	1.516	−9.285	9440	3.201	3.828401	−0.6274
4	1.506	−9.047	11658	3.934	4.135302	−0.2013
5	1.576	−9.481	11730	4.638	4.340598	0.297 402
6	1.589	−9.360	9456	4.098	4.008318	0.089 682
7	1.492	−9.432	7498	3.556	3.479906	0.076 094
8	1.652	−8.738	18918	5.603	5.586754	0.016 246
9	1.533	−9.018	20634	5.583	5.596253	−0.013 25
10	1.574	−4.106	14194	4.486	4.328855	0.157 145
11	1.675	−2.174	14254	4.14	4.436201	−0.2962
12	1.528	−3.517	14308	4.4	4.196114	0.203 886
13	1.548	−9.208	17276	5.0736	5.119924	−0.046 32
14	1.561	−7.062	17318	5.0749	5.001344	0.0735 56

test set. The following results were obtained:

(i) In the training set, a correlation of over 0.8 was obtained

(ii) In the test set, only a small decrease in correlation

$$\text{Toxicity} = -0.745 + 1.08026\text{Ch}_{DBF} + 0.4265C_{(LM\_W\_CJD_e\_SGI)} \quad (19)$$

$$R^2 = 0.888, n = 16, F = 51.704, s = 0.493$$

was seen ($R_{cv}^2 = 0.854$) and there was also a small increase in the standard error of the estimate ($s = 0.574$). This indicates that the model is valid. A plot of the observed versus calculated toxicity of dibenzofurans is given in Figure 3. Since the biological response is multiconditional, our results are statistically significant, and the descriptor weighted by the chemical nature of atoms functions correctly in the above model. The above results can be compared with the best one reported by Basak:[50] $R_{cv}^2 = 0.862$, in four variables.

5.3. Resonance Energy of Polyhexes. Two sets of polyhex structures have been selected.[54] The first consists of pyrene derivatives (Table 14); the other comprises polyhexes related to coronene (Table 15), and the modeled property was the resonance energy. Compared to the time-consuming ab initio density functional theory or even semiempirical calculations, some easily calculated descriptors such as the Cluj descriptors could be attractive in predicting, with a lower computational cost and adequate accuracy, the resonance energy of such molecules. Even a clearly nonlinear size dependence of the quantum parameter was recognized. In this context, the good correlations reported here are only a rough measure of the size effect inferred here. No direct comparable studies on these sets are available.

Table 16 lists data for the pyrenic structures from Table 14. Only Cluj descriptors have been used. The correlation is shown in Figure 4.

In the case of the structures formally derived from coronene (Tables 15 and 17), an initial correlation was made on 14 structures. In addition to the Cluj descriptors, we used the I_{Ω} index, calculated on the Omega polynomial, and the value of the highest occupied molecular orbital (HOMO) orbital, calculated at the PM3 level of theory. The correlation is given in eq 20

$$\text{RE} = -1.883\ 25 + 2.350\ 69I - 0.0728\text{HOMO} + 0.000\ 156UCJDI_p \quad (20)$$

$$n = 14, R^2 = 0.9144, F = 35.628, s = 0.2731$$

Compound 3 (Table 15) had a residual value, res = 0.6274, twice larger than the standard error (*s*), and this structure (or its RE value) was considered to be an outlier and was removed from the set. The equation calculated using the remaining 13 molecules revealed better statistics (eq 21), thus proving that molecule #3 is an outlier

$$\text{RE} = -0.8057 + 1.703\ 954I_{\Omega} - 0.077\ 25\text{HOMO} + 0.000\ 152UCJDI_p$$

$$n = 13, R^2 = 0.9609, F = 73.821, s = 0.1775 \quad (21)$$

The plot of resonance energy against that calculated by eq 21 is given in Figure 5.

The topological descriptors used in this work were calculated with our original software.[30,55,56]

6. CONCLUSIONS

A novel class of counting polynomials, called Cluj polynomials, has been proposed on the basis of the previously described Cluj matrices.

It was shown that the polynomial coefficients can be calculated from the Cluj matrices or by means of orthogonal edge cuts in the case of the $CJDI_e$ version. Analytical formulas for calculating the Cluj and related polynomials in phenylenes, spiranes, pyrenes, and coronenes have been developed.

Basic definitions and properties of the Cluj matrices and corresponding polynomials are given. The meaning of the Cluj descriptors, as vertex proximity descriptors, is demonstrated. For $CJDI_e$, it was shown that, in bipartite graphs, the sum of all edge-counted vertex proximities equals the product $v \times e$ of the number of vertices and edges in the graph. In trees, the sum of all path-counted vertex proximities is twice the Wiener index.

The relationship of Cluj polynomials $CJDI(G,x)$ with $\Omega(G,x)$ and $N\Omega(G,x)$ polynomials is described. The descriptors derived from the Cluj and related polynomials were used to predict the boiling point, chromatographic retention index, and resonance energy of sets of planar polyhex structures. The use of vertex proximity calculations in evaluating the bond polarity and molecular dipole moments was suggested. The toxicity of polychlorinated dibenzofurans was modeled by using an autocorrelated synthetic index derived from partial charges of atoms and added to a Cluj descriptor. The Cluj and related polynomial descriptors proved to be useful

tools in quantitative structure–property relationship/quantitative structure–activity relationship studies.

ACKNOWLEDGMENT

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