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It is intended that the journal may act as an interdisciplinary forum for publishing chemically important mathematical papers. Papers published in this journal must have a clear connection to chemistry with non-trivial mathematics.

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Hypercube Related Polytopes

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Body centered structures are used as seeds for a variety of structures of rank 3 and higher. Rhombellane structures are introduced and their design and topological properties are detailed.

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1 INTRODUCTION

A regular polyhedron is a polyhedron having congruent regular polygons as faces, arranged in the same manner around identical vertices; its symmetry group acts transitively on its flags, a regular polyhedron being vertex-, edge- and face-transitive [1]. They show three symmetry groups: *tetrahedral*; *octahedral* (or cubic) and *icosahedral* (or dodecahedral). Any shapes with icosahedral or octahedral symmetry will also include the tetrahedral symmetry.

There are five regular polyhedra, known as Platonic polyhedral solids: *tetrahedron* (T), *cube* (C), *octahedron* (O), *dodecahedron* (D) and *icosahedron* (I), written as {3,3}; {4,3}; {3,4}; {5,3} and {3,5} by using the basic Schläfli [2] symbols {p,q} where *p* is the number of vertices in a given face while *q* is the number of faces containing a given vertex.

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They show pair duals: (cube & octahedron) and (dodecahedron & icosahedron) while the tetrahedron is selfdual.

Generalization of a polyhedron to *n*-dimensions is called a polytope [1,3]. Regular 4-polytopes are written as $\{p,q,r\}$ and have cells of the type $\{p,q\}$, faces $\{p\}$, edge figures $\{r\}$ and vertex figures $\{q,r\}$; it means that *r*-polyhedra (of the type $\{p,q\}$) meet at any edge of the polytope. There are six regular 4-polytopes: 5-cell {3,3,3}; 8-cell {4,3,3}; 16-cell {3,3,4}; 24-cell {3,4,3}; 120-cell {5,3,3} and 600-cell {3,3,5}. Five of them can be associated to the Platonic solids but the sixth, the 24-Cell has no 3D equivalent. Among them, 5-cell and 24-cell are selfduals while the others are pairs: (8-cell & 16-cell); (120-cell & 600-cell).

A 5-polytope is written as $\{p,q,r,s\}$, where $\{p,q,r\}$ is the 4-face type, $\{p,q\}$ is the cell type, $\{p\}$ is the face type; $\{s\}$ is the face figure, $\{r,s\}$ is the edge figure and $\{q,r,s\}$ is the vertex figure. The three types of convex regular polytopes in dimensions 5 and higher, are as follows.

The *n-simplex* [1,4], with the Schläfli symbol $\{3^{n-1}\}$, and the number of its *k*-faces $\binom{n+1}{k+1}$; it is a generalization of the triangle or tetrahedron to *n*-dimensions. A regular *n*-simplex may be constructed from a regular $(n-1)$-simplex by connecting a new vertex to all original vertices.

The *hypercube* Q_n is a generalization of the 3-cube to *n*-dimensions; it has the Schläfli symbol $\{4,3^{n-2}\}$ and the number of *k*-faces given by $2^{n-k}\binom{n}{k}$. The hypercube can be constructed by the Cartesian product graph of *n* edges: $(P_2)^{\square n} = Q_n$; the Q_4 hypercube is called 8-cell or also tesseract.

The *n-orthoplex* or cross-polytope [1] has the Schläfli symbol $\{3^{n-2},4\}$ and *k*-faces $2^{k+1}\binom{n}{k+1}$; it is the dual of *n*-cube. The cross-polytope faces are simplexes of the previous dimensions, while its vertex figures are other cross-polytopes of lower dimensions.

For general surfaces, Euler [5] characteristic χ can be calculated as an alternating sum of figures of rank *k* [6–8]:

$$\chi(S) = f_0 - f_1 + f_2 - f_3 + ...,$$

It may be used for checking the consistency of a proposed structure.

An abstract polytope is a structure which considers only the combinatorial properties of a classical polytope: angles and edge lengths are disregarded. No space, such as Euclidean space, is required to contain an abstract polytope [7], which is a partially ordered set (poset). Every polytope has a dual, of which partial order is reversed; the dual of a dual is isomorphic to the original. A polytope is self-dual if it is the same as (*i.e.* isomorphic to) its dual. Any abstract polytope may be realized as a geometrical polytope having the same topological structure.

[1,1,1]Propellane is an organic molecule, first synthesized in 1982 [9]; by *IUPAC* rules, it is named tricyclo[1.1.1.$0^{1,3}$]pentane, a hydrocarbon with formula C_5H_6. The length of central bond separating the triangles is 160 pm, much longer than 154 pm, the average length of sp^3 C-C bond; this bond may be considered non-effective and the propellane consisting of squares/rhombs, a triangle-free structure.

Rhombellation is a procedure enabling the design of generalized rhombellanes, performed as follows: join by a point (called “rbl-point”) the two vertices lying opposite diagonal in each rhomb of an all rhomb-map (considered the zero-generation, Rh_0). Then, add new vertices opposite to the parent vertices and join each of them with the rbl-vertices lying in the proximity of each parent vertex, thus local Rh-cells being formed. The process can continue, considering the envelope Rh_n as “Rh_0” for Rh_{n+1}, in this way shell by shell being added to the precedent structure. Since the two diagonals may be topologically different, each generation may consist of two isomers.

Proposition [10]. *A structure is a rhombellane if all the following conditions are obeyed:*

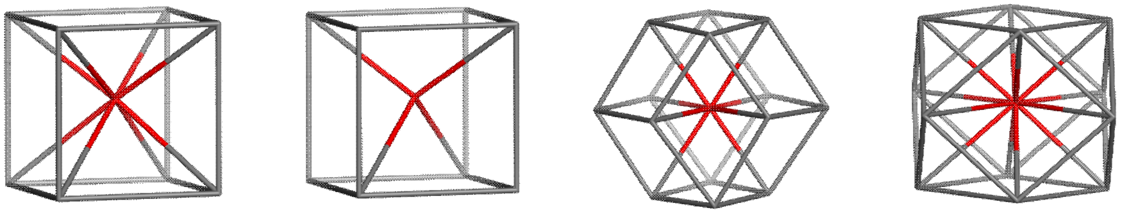
- *a) All strong rings are squares/rhombs;*
- *b) Vertex classes consist of all non-connected vertices;*
- *c) Omega polynomial has a single term: 1X^|E|;*
- *d) Line graph of the original graph shows a Hamiltonian circuit*;
- *e) Structure contains at least one* $K_{2.3}$ *subgraph.*

A fast detected condition is $\Omega(x) = 1x^e$, in words: all the edges in G are topologically parallel. Omega polynomial is defined as: $\Omega(x) = \Sigma_s m x^s$, m being the number of opposite edge strips, *ops*, of length s, in a graph G. There are graphs with a single *ops*, which is a Hamiltonian circuit. For such graphs, omega polynomial has a single term: $\Omega(x) = 1x^s$; $s = e = |E(G)|$. Hamiltonicity is an *np*-complete problem, being here a corollary of a single *ops* in the omega polynomial; however, not any graph having a Hamiltonian circuit has all the edges topologically parallel (see the case of cube and cuboctahedron). By construction, the rhombellanes have all classes of vertices not connected to each other within a same class. The smallest rhombellane is $K_{2.3}$, *i.e.*, the complete bipartite graph (corresponding to the [1,1,1]propellane molecule); any $K_{2.n}$ graph fulfills all the above conditions. A $K_{2.n}$ graph consists of $n(n\text{-}1)(n\text{-}2)/6$ $K_{2.3}$ substructures. There are graphs with more than two vertex classes obeying the above conditions; the proposed rhombellation operation enables the design of such graphs.

Rhombellanes represent *n*-partite graphs, both by topology and coloring [11,12]. Some crystal networks also fulfill the above criteria; among these, only the *dia* net is full rhombellanic.

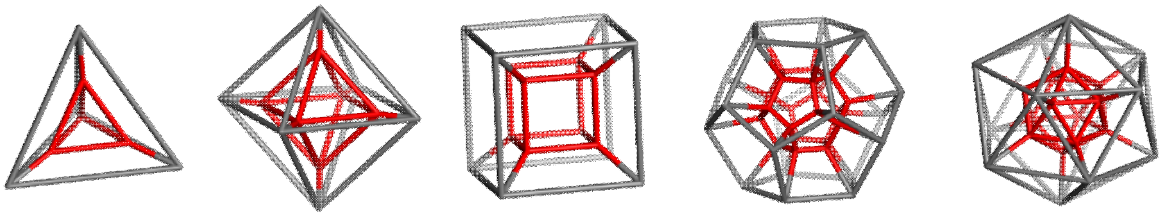
2 BODY–CENTERED CLUSTERS

Body centered clusters, derived from the Platonic solids (here denoted by MP^n), represent cell-duals of polyhedra having *n*-cells around a central cell; they are objects of Euclidean 4D-space [13]; this idea can be extended to objects other than Platonics (Figure 1); extension of P central point to a same cell leads to “cell-in-cell” clusters (Figure 2). Such body centered clusters have been used to design a plethora of polyhedral or non-polyhedral objects, and also periodic networks [14].



CP^8.9 (*bcu*) CP^4.9 (*dia*) Rh$_{12}$P^8.15 (*bcu*) COP^{12}.13 (*fcu*)

Figure 1. Seeds for some periodic networks.



T@T.8 O@O.12 C@C.16 D@D.40 I@I.24

Figure 2. Cell-in-cell clusters of the Platonic solids.

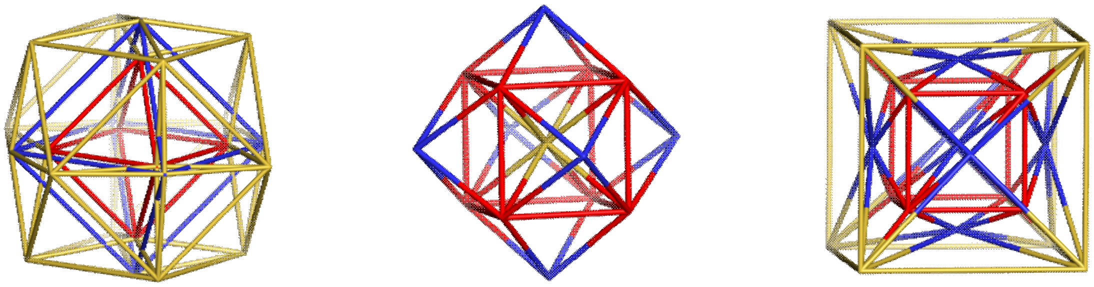
3. THE 24–CELL

The 24-cell (Figure 3, left) is a convex regular 4-polytope, also called “icositetrachoron”, “octaplex”, or polyoctahedron”, as it consists of 24 octahedral cells, with six of them meeting at each vertex and three at each edge; its vertex figure is a cube. The 24-cell is the unique self-dual regular polytope, (of which dual is) neither a polygon nor a simplex; by this reason, it has no analogue in 3D.

The vertex figure at a given vertex comprises all the figures incident on that vertex; edges, faces, etc. A vertex figure of an *n*-polytope is an ($n-1$)-polytope (*e.g.*, the vertex figure of a 4-polytope is a 3-polytope, or a polyhedron) [14].

The first 8 vertices of 24-cell are the vertices of a regular 16-cell while the remaining 16 are the vertices of the dual 8-cell, or the tesseract, Q_4.16. This suggests the construction either by *rectification* of 16-cell (*i.e.*, *medial* *m*(16-cell)) or by *dualization* of 8-cell (*i.e.*, *d*(8-cell)). There are several 3D projections of 24-cell, of which envelopes are the rhombic dodecahedron Rh_{12}, cuboctahedron CO, hexagonal bi-antiprism, elongated hexagonal bipyramid or a tetrakis hexahedron (*i.e.*, stellated cube *st*(C) – Figure 3, middle).

Starting from the idea of MP^n clusters, and keeping in mind the projection of 24-cell with a *st*(C) envelope, a construction of 24-cell as all-body-centered hypercube $Q_4.8CP^8.24$ is proposed here, by joining eight CP^8 units (Figure 3, right). In our best knowledge, this construction was not yet reported in literature.



24-Cell.24
Cuboctahedron
orthogonal projection

$st(CP^8).15$

$Q_4.8CP^8.24$

Figure 3. 24-Cell appearance.

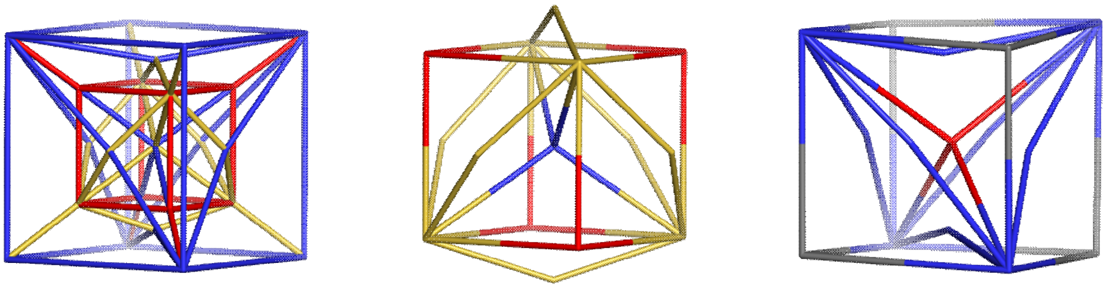
The figure count and topology sequence for $Q_4.8CP^8.24$ are given in Tables 1 and 2, respectively. As can be seen, both CP^8 and $Q_4.8CP^8.24$ have the rank $k = 4$. There is a single class of vertices in 24-cell, thus a single sequence of connectivity (provided by the layer matrix of connectivity LC) and rings around vertices (in terms of layer of rings LR) will fully describe its topology [15,16]. Omega polynomial [17,18] Ω = 96X^1 shows that there are 96 f_3 (*i.e.*, triangles), counted as non-topologically parallel 96 edges. It means that 24-cell is not a Rhombellane (cf. Proposition).

Table 1. Figure count in Q_4 related structures.

Polytope	v	e	f_3	f_4	f_6	2	$K_{2.3}$	$K_{2.4}$	Ada(Py_4)	3	4	χ	k
CP^8	9	20	12	6	0	18	0	0	(6)	7	-	0	4
$Q_4.8CP^8$	24	96	96	0	0	96	0	0	0	24	-	0	4
CP^4	9	16	0	18	0	18	10	0	0	11	-	0	4
$Q_4.8CP^4$	24	64	0	120	8	128	80	12	2	94	8	2	5

4. A RHOMBELLANIC HYPERCUBE RELATIVE

By deleting, in an alternating manner, four edges incident at each central point in $Q_4.8CP^8.24$ it results in a new structure, $Q_4.8CP^4.24$ (Figure 4), which is a rhombellane relative of the hypercube Q_4 (see below). The repeating unit is now $CP^4.9$, a 4-polytope ($k = 4$, see Table 1); it consists of ten simplest rhombellanes $K_{2.3}$. There are eight CP^4 facets (of rank $k = 4$) binding $Q_4.8CP^4.24$; each pair of CP^4 facets shares a facet of rank $k = 3$, namely the rhombellane $K_{2.4}$; thus, $Q_4.8CP^4.24$ is a 5-polytope ($k = 5$). In the figure count, two adamantine *ada* units ($k = 3$) and eight hexagons f_6 were considered (Figure 4, middle and right); adamantane is not a polyhedron but a tile [19], similar to rhombellanes, from which it originates. Sequences of $Q_4.8CP^4.24$ topology are given in Table 2. There are two vertex classes, of degree 4 {16} and 8 {8}, respectively. Omega polynomial consists of a single term, Ω = 1X^64, saying that the edges of $Q_4.8CP^4.24$ are all topologically parallel and thus the structure is a rhombellane. The vertex classes have all non-connected points (as a bipartite structure), an additional proof supporting the rhombellanic nature of this structure of higher rank. About centrality, counted by our centrality index [15], the 16 points class appears lying more central (C=0.1256396237) than the remaining 8 vertices (C= 0.1203238919). Computations have been done by our Nano-Studio software program [20].



$Q_4.8CP^4.24$ Ada.CP^4.15 (inside) Ada.CP^4.15 (outside)

Figure 4. A rhombellanic hypercube Q_4 relative (left); details of its inside (middle) and outside (right).

Table 2. Sequence of connectivity (LC) and rings around vertex (LR) in all-centered 8-Cell (Tesseract) $Q_4.8CP^n.24$.

Polytope	LC	LR	Ω	Degree	Rings
$Q_4.8CP^8.24$					
24 ×	1 - 8 - 14 - 1	12 - 96 - 168 - 12	96X^1	8	3^12
$Q_4.8CP^4.24$					
16 ×	1 - 4 - 14 - 4 – 1	18 - 144 - 252 - 144 – 18	1X^64	4	4^18
8 ×	1 - 8 - 6 - 8 - 1	36 - 144 - 216 - 144 - 36		8	4^36

5. CONCLUSION

The smallest rhombellane, [1,1,1]propellane, is a real chemical molecule; its associate graph is the complete bipartite graph, $K_{2.3}$. Generalized rhombellanes are designed by Diudea's rhombellation procedure. Rhombellanes have all the edges topologically parallel, as shown by the single term in Omega polynomial (further involving Hamiltonian circuits visiting their edges). Rhombellanes consist of at least one $K_{2.3}$ subgraph.

A new building way for the 4-polytope, 24-cell, from all-P^8 body centered hypercube Q_4 was proposed. Its P^4 analogue, $Q_4.8CP^4.24$, is a 5-polytope.

Structure representation in terms of small rhombellanes brings more structural insight and may unveil relations among structures apparently not related. Rhombellanes represent a new class of structures, with interesting properties, both in theory and applications.

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General Theory of Cycle–Dependence of Total π–Electron Energy

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ABSTRACT

The theoretical treatment of cycle-effects on total π-electron energy, mainly elaborated by Nenad Trinajstić and his research group, is re-stated in a general and more formal manner. It enables to envisage several other possible ways of measuring the cycle-effects and points at further directions of research.

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1. INTRODUCTION: MATHEMATICAL BACKGROUND

Let G be a graph representing the carbon–atom skeleton of a polycyclic conjugated π-Electron system [7,9,21,34]. In what follows, we refer to G as to a molecular graph. Let G possess a total of $t = t(G)$ cycles, and let these cycles be denoted by $Z_1, Z_2, ..., Z_t$.

In order to avoid any misunderstanding, in Fig 1 are indicated all the cycles contained in the molecular graph of triphenylene G_{TP}. Thus, although G_{TP} is classified among tetracyclic graphs (i.e., G_{TP} has 4 independent cycles), it possesses a total of 11 cycles, $t(G_{TP}) = 11$.

In theoretical chemistry, it has been firmly established that the cycles in conjugated molecules have a profound influence on their physical and chemical properties, especially on those that are referred to as “aromaticity” and “local aromaticity” [27,6,30,28,13].

The considerations that follow are intimately related with the Sachs theorem and Its role in quantum chemistry. This theorem was published in its final form by Horst Sachs

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in 1964 [29], but remained fully unknown to the chemical community until the publication of the paper in 1972 [8]. Details of the Sachs theorem can be found in scores of books and review articles, for instance in [23,32,31,9,34,21,7,16]; for historical details see [11,12,35].

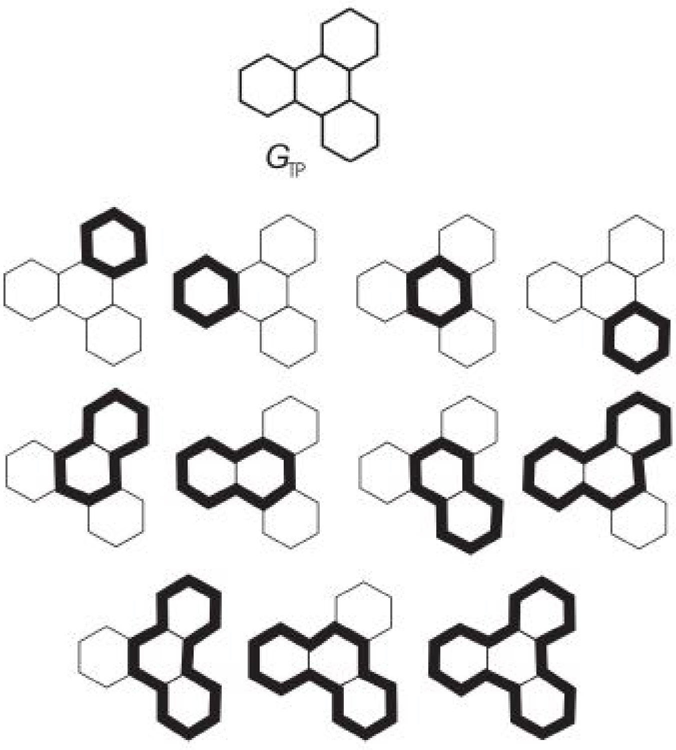

Figure 1. The molecular graph G TP of triphenylene and the cycles contained in it.

Let G be a molecular graph and ϕ(G,λ) its characteristic polynomial. Let G has n vertices, which means that ϕ(G,λ) is a monic polynomial of degree n.

A Sachs graph S is any graph whose components are cycles and/or 2-vertex Complete graphs. Denote by n(S), p(S), and c(S) the number of vertices, number of components, and number of cyclic components, respectively of the Sachs graph S. Denote by S(G) the set of all Sachs graphs that are as subgraphs contained in the graph G. Then the Sachs theorem reads,

$$\phi(G,\lambda) = \lambda^n + \sum_{S\in S(G)} (-1)^{p(S)}\, 2^{c(S)} \lambda^{n-n(S)} \tag{1}$$

Important for the present consideration is that the Sachs theorem relates the Characteristic polynomial with the structure of the underlying graph. Furthermore, it clearly and explicitly shows how the characteristic polynomial depends on the cycles Contained in the graph.

By solving the equation $\phi(G,\lambda) = 0$, one obtains the eigenvalues of the graphs G, denoted by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Within the framework of the tight-binding Hüuckel molecular orbital (HMO) approximation, the total π-electron energy of the underlying conjugated molecule can then be calculated as [9, 21]

$$E(G) = \sum_{i=1}^{n} \omega_i \lambda_i \tag{2}$$

where ω_i is the occupation number of the i-th molecular orbital, $\omega_i \in \{0,1,2\}$. Thus, the Sachs theorem in an implicit manner reveals how the total π-electron energy depends on the cycles contained in the molecular graph.

In order to measure the effect of cycles, a quasi-energy E(G,ref) needs to be constructed in an analogous manner as E(G), using not the zeros of the characteristic polynomial, but the zeros of a suitably constructed “reference polynomial”. Then the difference $E(G) - E(G,ref)$ provides a desired measure of the respective energy-effect, and can be directly related with the physical and chemical properties of the underlying conjugated π-electron systems.

2. MODELING THE ENERGY–EFFECTS

Let Z_1, Z_2, ..., Z_t be the cycles contained in the molecular graph G. For i = 1,2,...,t, associate a variable g_i to the cycle Z_i . Let $g = (g_1, g_2, ..., g_t)$ be a t-dimensional vector. If $g_1 = g_2 = \cdots = g_t = 0$, then we write g = 0. If $g_1 = g_2 = \cdots = g_t = 1$, then g = 1. By e_i we denote the g-vector in which all components are equal to zero, except the i-th component, which is equal to unity. Thus, $g = \sum_{i=1}^{n} g_i e_i$.

Bearing in mind Eq. (1), we define an auxiliary polynomial

$$\phi(G,g,\lambda) = \lambda^n + \sum_{S \in S(G)} (-1)^{p(S)}\, 2^{c(S)} Z(S)\, \lambda^{n-n(S)}$$

where Z(S) is the product of g_i-values of all cycles contained in the Sachs graph S. If the Sachs graph S is acyclic, then Z(S) = 1.

It is evident that $\phi(G,1,\lambda) \equiv \phi(G,\lambda)$, i.e., $\phi(G,1,\lambda)$ coincides with the ordinary characteristic polynomial. In addition, $\phi(G,0,\lambda)$ is equal to the matching polynomial, whose theory has been studied in due detail [5,15].

By solving the equation $\phi(G,g,\lambda) = 0$, one obtains the quasi-eigenvalues $\lambda_1(g)$, $\lambda_2(g)$, ..., $\lambda_n(g)$. Based on them, it is possible to compute a quasi-energy E(G,g) in the same manner as the total π-electron energy E(G) is calculated from the ordinary graph eigenvalues (as specified in the preceding section). Then, in particular, E(G,1) coincides with the ordinary total π-electron energy E(G), Eq. (2).

The quasi-energy E(G,g) has to be understood as a total-π-electron-energy-like quantity, in which the parameter g_i controls the effect of the i-th cycle contained in the molecular graph. If $g_i = 1$, then the effect of this cycle of total π-electron energy has the usual, normal value. If $g_i = 0$ then the effect of the i-th cycle is completely neglected.

Based on this simple observation, by means of the difference E(G,1) − E(G,g), and by a pertinent choice of the g-vector, it was possible to extract a variety of chemically relevant information contained in the HMO total π-electron energy. In what follows, we list a few such cases that earlier have been studied in the chemical literature. In the subsequent section, we point out other options that our general Theory makes possible.

2.1. THE TOPOLOGICAL RESONANCE ENERGY

Using the above introduced formalism, the "it topological resonance energy" is defined as

$$\mathrm{TRE}(G) = E(G,1) - E(G,0) \tag{3}$$

It represents the effect on total π-electron energy of all cycles contained in the molecular graph G. This idea was first put forward in 1975 by Nenad Trinajstić and two of his students [18], and eventually elaborated in 1977, in the papers [33,19]. In the same time Aihara arrived at the very same idea [1]. Details and an extensive bibliography of the theory and numerous applications of the TRE model can be found in the survey [14], whereas a few interesting historical data in Trinastić's autobiography [35].

2.2. MODELS OF ENERGY−EFFECT INDIVIDUAL CYCLES

Whereas TRE represents the simultaneous effect of all cycles of total π-electron energy, an analogous reasoning lead to the expression

$$ef(G,Z_i) = E(G,1) - E(G,1-e_i) \tag{4}$$

which would provide a measure of the effect of the individual cycle Z_i. This model was proposed in 1977, in the paper [4]. The idea came from Gutman, whereas Slobodan Bosanac provided the software by means of which the ef-values could be efficiently calculated. The first chemical applications of this model were communicated in [17], and were followed by many dozens of publications; mathematical details and bibliography can be found in the survey [13].

In the same year 1977, Aihara introduced an alternative model for measuring the energy-effect of individual cycles [2]. In our symbolism, this energy-effect can be expressed as

$$ef_A(G,Z_i) = E(G,e_i) - E(G,0) \tag{5}$$

In the case of unicyclic graphs, $ef_A(G) = ef(G)$, whereas in the case of graphs with more than one cycle, the two ef-values differ. Worth mentioning is that for all graphs G and all i = 1,2,...,t, the quasi-eigenvalues $\lambda_1(e_i)$, λ_2 (e_i), ..., $\lambda_n(e_i)$, i.e., the zeros of the polynomial $\beta(G,Z_i,\lambda) = \phi(G,e_i,\lambda)$ are all real-valued. This fact was first established on a large number of examples [24,25] and eventually proved for the general case [26].

In a later article [3], Aihara himself came to the conclusion that the ef-model, Eq. (4), is superior to its ef A -version, Eq. (5).

Formula (4) can be directly extended to measure the collective energy-effect of a pair of cycles Z_i, Z_j, $ef(G, Z_i, Z_j) = E(G, 1) - E(G, 1 - e_i - e_j)$ of a triplet of cycles Z_i ,Z_j, Z_k , $ef(G, Z_i, Z_j, Z_k) = E(G, 1) - E(G, 1 - e_i - e_j - e_k)$ etc. However, to the present author's best knowledge, these multiple-energy-effects have been considered in just a single paper [22].

3. MORE POSSIBILITIES OF THE GENERAL THEORY

The choice $g = 1 - e_i$ in Eq. (4) means that we completely neglect the influence of the cycle Z_i on the value of the quasi-energy $E(G,g)$. Analogously, the choice $g = 0$ in Eq. (3) means that we completely neglect the influence of all cycles on the value of the quasi-energy $E(G,g)$.

However, we may only partially diminish the effect of cycles (by choosing $0 < g_i < 1$). In this case, a resonance energy of the form,

$$TRE_a(G, \varepsilon) = \frac{1}{\varepsilon}[E(G, 1) - E(G, (1 - \varepsilon)1)]$$

would be conceived, in which case $TRE_a(G,\varepsilon) = TRE(G)$ if $\varepsilon = 1$. For instance, by setting $\varepsilon = 1/2$, we would get a kind of "half-way" resonance energy. Anyway, ε could be viewed as a variable parameter, whose value could then be optimized (so that TRE_a best agrees with experimentally observed facts).

Another development beyond the standard TRE model would be to increase the effect of cycles above their usual value. The resonance energy obtained in this way would be,

$$TRE_b(G, \varepsilon) = \frac{1}{\varepsilon}[E(G, (1 + \varepsilon)1) - E(G, 1)] \tag{7}$$

in which case $TRE_b(G,\varepsilon) = TRE(G)$ if $\varepsilon = -1$. It can be shown that

$$\lim_{\varepsilon \to 0} TRE_a(G, \varepsilon) = \lim_{\varepsilon \to 0} TRE_b(G, \varepsilon) = \frac{\partial E(G, x1)}{\partial x} |x = 1 \tag{8}$$

The partial derivative on the right–hand side of (8) was earlier studied in [10,20], where it was shown to be equal to the sum of contributions of individual cycles contained in the molecular graph G.

Analogous extensions could be done also with the individual energy-effect ef(G), Eq. (4). Thus, one might consider

$$ef_a(G, Z_i, \varepsilon) = \frac{1}{\varepsilon}[E(G, 1) - E(G, 1 - \varepsilon e_i)] \tag{9}$$

or

$$ef_b(G, Z_i, \varepsilon) = \frac{1}{\varepsilon}[E(G, 1 + \varepsilon e_i) - E(G, 1)] \tag{10}$$

which evidently become equal to ef(G,Z_i) for $\varepsilon = +1$ and $\varepsilon = -1$, respectively. In connection with this, it can be shown that,

$$\lim_{\varepsilon\to 0} ef_a(G,Z_i,\varepsilon) = \lim_{\varepsilon\to 0} ef_b(G,Z_i,\varepsilon) = \frac{\partial E(G,g)}{\partial g_i}|g = 1.$$

4. CONCLUDING REMARKS

The fact is that the variable-parameter energy-effects defined via Eqs. (6) , (7), (9) , (10), and similar have never been studied in theoretical chemistry. Their "ordinary" versions, Eqs. (3)–(5), were put forward in the 1970s, when the interest for HMO-based aromaticity criteria might have been at a maximum. In the meantime, the usage of HMO-based theories gradually lost their attractiveness, and nowadays it is unlikely that the models mentioned in the preceding section will be further elaborated and attempted to find chemical applications. Therefore, the present paper should be considered as a summary of what the research group of Nenad Trinajstić achieved in the study of cycle-effects in polycyclic conjugated molecules, and what could have had achieved, but did not. Sincere congratulations and best wishes to N.T.'s 80th birthday.

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More Inequalities for Laplacian Indices by Way of Majorization

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ABSTRACT

The n-tuple of Laplacian characteristic values of a graph is majorized by the conjugate sequence of its degrees. Using that result we find a collection of general inequalities for a number of Laplacian indices expressed in terms of the conjugate degrees, and then with a maximality argument, we find tight general bounds expressed in terms of the size of the vertex set n and the average degree $d_G = 2|E|/n$. We also find some particular tight bounds for some classes of graphs in terms of customary graph parameters.

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1. INTRODUCTION

Let $G = (V, E)$ be a finite simple connected graph with vertex set $V = \{1, 2, \ldots, n\}$, degrees $d_1 \geq d_2 \geq \cdots \geq d_n$, and $d_G = \frac{2|E|}{n}$ the average degree. Let A be the adjacency matrix of G, D the diagonal matrix having the degrees of G in its diagonal and $L = D - A$ the Laplacian matrix of G, with characteristic values $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} \geq \lambda_n = 0$. There exist many indices in Mathematical Chemistry expressed in terms of these characteristic values that we shall look at; among them the *Laplacian energy like invariant* put forward in [13]:

$$LEL(G) = \sum_{i=1}^{n-1} \sqrt{\lambda_i}, \tag{1}$$

and its generalization (see [4], [7])

$$LEL_\beta(G) = \sum_{i=1}^{n-1} \lambda_i^\beta \tag{2}$$

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for arbitrary $\beta \neq 0{,}1$; we shall also be concerned with the Kirchhoff index (see [12]) $R(G) = \sum_{i<j} R_{ij}$, where R_{ij} represents the effective resistance, as computed by Ohm's and Kirchhoff's laws, between the vertices i and j, and equal also to (see [8] and [18])

$$R(G) = n\sum_{i=1}^{n-1}\frac{1}{\lambda_i}. \tag{3}$$

We shall also discuss the Laplacian energy put forward in [9] as

$$LE(G) = \sum_{i=1}^{n}|\lambda_i - d_G|. \tag{4}$$

And finally we will consider the Laplacian Resolvent Energy of a graph, proposed by Cafure et al. in [3] as an alternative to the Resolvent Energy (see [11]) defined as

$$RL(G) = \sum_{i=1}^{n}\frac{1}{n+1-\lambda_i}. \tag{5}$$

The main ideas around majorization (for more details the reader is referred to [14]) may be briefly exposed thus: for any n-tuples $x = (x_1, \ldots, x_n)$ and $y = (y_1, \ldots, y_n)$ with $x_1 \geq x_2 \geq \ldots \geq x_n$ and $y_1 \geq y_2 \geq \ldots \geq y_n$, x majorizes y, written $x \succ y$, if

$$\sum_{i=1}^{k} x_i \geq \sum_{i=1}^{k} y_i, \tag{6}$$

for $1 \leq k \leq n-1$ and

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i, \tag{7}$$

A real function $\Phi : \mathbb{R}_n \to \mathbb{R}$ is a Schur-convex function in case it maintains the majorization inequality, that is, if $\Phi(x) \geq \Phi(y)$ whenever $x \succ y$. Similarly, a Schur-concave function inverts the inequality: $\Phi(x) \leq \Phi(y)$ whenever $x \succ y$. A Schur-convex (resp.Schur-concave) function can be simply constructed considering $\Phi(x) = \sum_{i=1}^{n} f(x_i)$, for any one-dimensional convex (resp. concave) real function $f : \mathbb{R} \to \mathbb{R}$.

The main idea for finding bounds through majorization for a molecular index is to express such index as a Schur-convex or Schur-concave function, and then to identify maximal and minimal elements, x^* and x_* respectively, that is, elements in the subspace of interest of the n-dimensional real space (which can be a set of n-tuples of degrees of vertices, or eigenvalues, or effective resistances, etc.) such that $x^* \succ x \succ x_*$, for all n-tuples x in the subspace of interest, and then if Φ is Schur-convex we will have $\Phi(x^*) \geq \Phi(x) \geq \Phi(x_*)$, for all x, having thus found the upper and lower bounds of interest, $\Phi(x^*)$ and $\Phi(x_*)$, respectively. A similar conclusion follows, exchanging the words ''upper" and "lower", if Φ is Schur-concave.

Several indices in Mathematical Chemistry such as (1), (2), (3), (4) and (5) are con-structed using Schur-convex or Schur-concave functions, and this fact has been used in a collection of articles (such as [2], [6], [13], [15], [16], for example) to find a cornucopia of upper and lower bounds for the indices. Specifically, in [15] we used the fact that the Laplacian eigenvalue sequence majorizes the degree sequence, i.e.:

$$(\lambda_1, \lambda_2, \ldots, \lambda_n) \succ (d_1 + 1, d_2, \ldots, d_n - 1), \tag{8}$$

with the purpose of finding lower (resp. upper) bounds, expressed in terms of the degree sequence, for descriptors defined through Schur-convex (resp. concave) functions.

Interestingly enough, there is a companion formula for (8), perhaps not so well known, where the eigenvalue sequence is majorized by another set of numbers, the conjugate degree sequence. In general, given a finite sequence $a_1, a_2, \dots, a_n$ of non-negative numbers, its conjugate sequence a $a'_1, a'_2, \dots, a'_n$ is defined by $a_j' = |\{i : a_i \geq j\}|$.

The conjugate sequence does not depend on the order of the original sequence and it is always a decreasing sequence, with $a_1' \leq n$ and $a_j' = 0$ for $j > max\{a_1, \dots, a_n\}$. For the sequence of degrees $d_1, \dots, d_n$ of any graph G it should be noted that we have $d_1' = n$ and $d_n' = 0$. For more details on conjugate sequences, the reader can consult [14].

Here is the important fact that was conjectured by Grone and Merris in [7] and that was finally proven by Bai in [1]:

Lemma 1. Given an arbitrary G we have

$$\left(d_1', \dots, d_n'\right) \succ (\lambda_1, \dots, \lambda_n) \tag{9}$$

It is clear that equation (9) (incidentally, since $d_n' = \lambda_n = 0$ this equation can be rewritten as $\left(d_1', \dots, d_{n-1}'\right) \succ (\lambda_1, \dots, \lambda_{n-1})$) can be used to find upper (resp. lower) bounds, in terms of the conjugate degree sequence, for Laplacian descriptors defined through Schur- convex (resp. concave) functions. This is precisely what Das et al. did in [5], where they worked with the Laplacian descriptors $LE(G)$ and $LEL(G)$, among other descriptors, and found some bounds in terms of the d_i's. In this article we will obtain additional bounds for the other Laplacian descriptors mentioned here in terms of the conjugate degree sequence, and then with a maximality argument used in majorization, we will find tight general bounds expressed in terms of the size of the vertex index n and the average degree d_G. We will also find some particular tight bounds given in terms of usual graph parameters.

2. THE INEQUALITIES

We begin with the general inequalities in the following

Proposition 1. For any G and $\{d_i'\}$ its conjugate degree sequence we have

$$LEL(G) \geq \sum_{i=1}^{n} \sqrt{d_i'}, \tag{10}$$

$$LEL_\beta(G) \leq \sum_{i=1}^{n-1} \left(d_i'\right)^\beta, \quad \text{for } \beta > 1 \text{ } or \text{ } \beta < 0 \tag{11}$$

$$LEL_\beta(G) \geq \sum_{i=1}^{n-1} \left(d_i'\right)^\beta, \quad \text{for } 0 < \beta < 1 \tag{12}$$

$$R(G) \le n\sum_{i=1}^{n-1}\frac{1}{d_i'}, \tag{13}$$

$$LE(G) \le \sum_{i=1}^{n-1}\left|d_i' - d_G\right| + d_G, \tag{14}$$

$$RL(G) \le \sum_{i=1}^{n-1}\frac{1}{n+1-d_i'} + \frac{1}{n+1}. \tag{15}$$

Proof. Apply (9) and the facts that $R(G)$, $LE(G)$, $LEL_\beta(G)$ for $\beta < 0$ or $\beta > 1$ and $RL(G)$ are Schur-convex, while $LEL(G)$ and $LEL_\beta(G)$ for $0 < \beta < 1$ are Schur-concave.

Inequality (10) was proven in [5]. One may ask how informative these inequalities are. For example, if any of the d_i's are zero, (13) provides no information. On the other hand, from the trivial observation that $d_i' \le n$, for $1 \le i \le n-1$, we can prove with a straightforward argument - worth comparing with the methods used in [17] and [3] to prove these facts - a couple of maximal results in the next

Proposition 2. For arbitrary G the following holds

$$LEL_\beta(G) \le LEL_\beta(K_n) = (n-1)n^\beta \quad \text{for} \quad \beta > 0, \tag{16}$$

and

$$RL(G) \le RL(K_n) = n - 1 + \frac{1}{n+1}. \tag{17}$$

Proof. Since the real functions $f(x) = x^\beta$ for $\beta > 0$ and $f(x) = \frac{1}{n+1-x}$ are increasing we obtain from (11) and (15) that $LEL_\beta(G) \le \sum_{i=1}^{n-1}(d_i')^\beta \le \sum_{i=1}^{n-1} n^\beta = (n-1)n^\beta$, and $RL(G) \le \sum_{i=1}^{n-1}\frac{1}{n+1-d_i'} + \frac{1}{n+1} \le \sum_{i=1}^{n-1} 1 + \frac{1}{n+1} = n - 1 + \frac{1}{n+1}$.

Since the Laplacian eigenvalues of the complete graph K_n are 0 and n with multiplicity $n-1$, it is readily seen that the equalities in (16) and (17) are attained by K_n.

We present now the following result, found in section 2.3 of [2] (corollary 2.3.2) as a lemma which will be used in the next proposition

Lemma 2. Let S_a be the set of real n-tuples $x = (x_1, x_2, \ldots, x_n)$ such that $x_1 \ge x_2 \ge \ldots \ge x_n$ and $\sum_{i=1}^{n} x_i = a$, which additionally satisfy $M \ge x_i \ge m$. Then the maximal element x^* of S_a, that is, the element such that for any other x we have $x^* \succ x$, is given by $x^* = (M, M, \ldots, M, \theta, m, m, \ldots, m)$, where M appears k times, m appears $n-k-1$ times, $k = \lfloor \frac{a-nm}{M-m} \rfloor$ and $\theta = a - Mk - m(n-k-1)$.

Now we can prove our main result in the following

Proposition 3. For any G we have

$$LEL(G) \ge \left(\lfloor d_G \rfloor + \sqrt{d_G - \lfloor d_G \rfloor}\right)\sqrt{n}, \tag{18}$$

$$LEL_\beta(G) \le [\lfloor d_G \rfloor + (d_G - \lfloor d_G \rfloor^\beta] n^\beta, \quad \text{for} \quad \beta > 1 \; or \; \beta < 0 \tag{19}$$

$$\mathrm{LEL}_\beta(G) \ge [\lfloor d_G \rfloor + (d_G - \lfloor d_G \rfloor^\beta] n^\beta, \quad \text{for} \;\; 0 < \beta < 1 \tag{20}$$

$$RL(G) \le \lfloor d_G \rfloor + \frac{1}{n(1-d_G+\lfloor d_G \rfloor)+1} + \frac{n-\lfloor d_G \rfloor - 1}{n+1}, \tag{21}$$

$$LE(G) \le 2\lfloor d_G \rfloor (n - d_G) \quad if \quad d_G \ge n(d_G - \lfloor d_G \rfloor). \tag{22}$$

$$LE(G) \le 2d_G(n - \lfloor d_G \rfloor - 1) \quad if \quad d_G \le n(d_G - \lfloor d_G \rfloor). \tag{23}$$

All the equalities in (18) through (22) are attained by the complete graph K_n

Proof. We prove only (22), since all the other inequalities have a similar proof. Consider the set $S_{2|E|}$ of all n-tuples $x = (x_1, x_2, \dots x_n)$ of non-negative numbers such that $\sum_i x_i = 2|E|$ and $n \ge x_i \ge 0$. With the notation of the lemma, $M = n$ and $m = 0$. Then $k = \lfloor \frac{2|E|}{n} \rfloor = \lfloor d_G \rfloor$ and $\theta = n(d_G - \lfloor d_G \rfloor)$. That means that the maximal element of $S_{2|E|}$ is $x^* = (n, n, \dots, n, n(d_G - \lfloor d_G \rfloor), 0, \dots, 0)$, where the coordinate n appears $\lfloor d_G \rfloor$ times. Since $x^* \succ (d_1', \dots, d_n')$ and the function that defines $LE(G)$ is Schur-convex, the following holds:

$$\begin{aligned} LE(G) &\le \textstyle\sum_{i=1}^{n} |d_i' - d_G| \le \sum_{i=1}^{\lfloor d_G \rfloor} (n - d_G) + |n(d_G - \lfloor d_G \rfloor) - d_G| + \sum_{i=\lfloor d_G \rfloor + 2}^{n} d_G \\ &= (n - d_G)\lfloor d_G \rfloor + |n(d_G - \lfloor d_G \rfloor) - d_G| + (n - \lfloor d_G \rfloor - 1) d_G \\ &= (\mathrm{n} - \mathrm{d_G})\lfloor \mathrm{d_G} \rfloor + d_G - n(d_G - \lfloor d_G \rfloor) + (n - \lfloor d_G \rfloor - 1) d_G \\ &= 2\lfloor d_G \rfloor (n - d_G). \end{aligned}$$

The reader may verify for the case of the complete graph K_n that both the value of $LE(K_n)$ and the upper bound are equal to $2(n - 1)$.

The following corollary is immediate from the previous proposition, but worth being expressed explicitly.

Corollary 1. If the average degree d_G is an integer then

$$LEL(G) \ge d_G \sqrt{n}, \tag{24}$$

$$LEL_\beta(G) \le d_G n^\beta, \quad \text{for} \; \beta > 1 \; or \; \beta < 0, \tag{25}$$

$$LEL_\beta(G) \ge d_G n^\beta, \quad \text{for} \; 0 < \beta < 1, \tag{26}$$

$$RL(G) \le \frac{n(d_G + 1)}{n+1}. \tag{27}$$

$$LE(G) \le 2d_G(n - d_G). \tag{28}$$

Remarks. The corollary holds, in particular, if the graph is d-regular. The proof of the lower bound (24), valid for all G, can be tracked down to [10]. Notice that our bound (18) is stronger than (24) in general, since

$$d_G\sqrt{n} = (\lfloor d_G \rfloor + d_G - \lfloor d_G \rfloor)\sqrt{n} \le (\lfloor d_G \rfloor + \sqrt{d_G - \lfloor d_G \rfloor})\sqrt{n},$$

because $0 \le d_G - \lfloor d_G \rfloor \le 1$. The same is valid for (20)–(22) with respect to (26)–(28). Of all these, perhaps the only one worth a couple of lines is the proof that (21) is always better than (27), and this, after some algebra is equivalent to proving that

$$\frac{1}{n^2(1-\alpha)\alpha + n + 1} \le \frac{1}{n+1}, \qquad (29)$$

for $\alpha = d_G - \lfloor d_G \rfloor$, which satisfies $0 \le \alpha \le 1$, and makes the truth of (29) obvious. As for (19), it is better than (25) only for $\beta > 1$.

In the next propositions, we explore other ways to handle the n-tuple of conjugate degrees that yield inequalities in terms of the usual graph parameters for certain classes of graphs.

Proposition 4. For a graph possessing k vertices with maximal degree $n - 1$ we have

$$LEL_\beta(G) \le n^\beta + (n-2)k^\beta \quad \text{for } \beta < 0, \text{ and } R(G) \le 1 + \frac{n(n-2)}{k}. \qquad (30)$$

The equalities in both cases are attained by the star graph S_n and the complete graph K_n .

Proof. We prove only the second half of (30) as the other proof is similar. We know that $d_1' = n$, and by the hypothesis $d_i' \ge k$ for $2 \le i \le n-1$. Given that the function $f(x) = \frac{1}{x}$ decreases in the interval $(0, \infty)$, by (13) we can write $R(G) \le n\left(\frac{1}{n} + \sum_{i=2}^{n-1}\frac{1}{k}\right) = 1 + \frac{n(n-2)}{k}$. In the case of the star graph it is well known that $R(S_n) = (n-1)^2$ which coincides with the upper bound when k = 1; in the case of the complete graph it is also well known that $R(K_n) = n - 1$ which coincides with the value of the upper bound when $k = n$.

Proposition 5. If G has k pendent vertices then

$$LEL_\beta(G) \le n^\beta + (n-2)(n-k)^\beta \text{ for } \beta > 1 \text{ and } RL(G) \le 1 + \frac{n-2}{k+1} + \frac{1}{n+1}. \qquad (31)$$

The equalities are attained by the star graph S_n

Proof. We prove the second half of (31). The hypothesis implies that $d_i' \le n - k$ for $2 \le i \le n-1$. Also the real function $f(x) = \frac{1}{n+1-x}$ is increasing, and therefore $RL(G) \le \sum_{i=1}^{n}\frac{1}{n+1-d_i'} = 1 + \sum_{i=2}^{n-1}\frac{1}{n+1-d_i'} + \frac{1}{n+1} \le 1 + \sum_{i=2}^{n-1}\frac{1}{n+1-(n-k)} + \frac{1}{n+1}$. Now for the n-star graph S_n its eigenvalues are $n, 1$ with multiplicity $n - 2$ and 0 and therefore $RL(S_n) = 1 + \frac{n-2}{n} + \frac{1}{n+1}$, which coincides with the upper bound when $k = n - 1$.

Proposition 6. If G is a chemical graph then

$$LEL_{\beta}(G) \leq 4n^{\beta}, \text{ for } \beta > 1 \text{ and } RL(G) \leq 4 + \frac{n-4}{n+1}. \qquad (32)$$

The equalities are attained by the complete graph K_5.

Proof. We prove the second half of (32). The hypothesis implies that $d_i^{'} \leq n$ for $1 \leq i \leq 4$ and $d_i^{'} = 0$ for $i > 4$. Therefore, with the same arguments as in the previous proposition $RL(G) \leq \sum_{i=1}^{n} \frac{1}{n+1-d_i^{'}} \leq \sum_{i=1}^{4} 1 + \sum_{i=5}^{n} \frac{1}{n+1} = 4 + \frac{n-4}{n+1}$. Combining the hypotheses of the last two propositions we obtain the next proposition with an obvious proof.

Proposition 7. If G is a chemical graph with k pendent vertices then

$$LEL_{\beta}(G) \leq n^{\beta} + 3(n-k)^{\beta}, \text{ for } \beta > 1 \text{ and } RL(G) \leq 1 + \frac{3}{k+1} + \frac{n-4}{n+1}.$$

The equalities are attained by the star graph S_5 .

3. CONCLUSIONS

The fact that the n-tuple of Laplacian eigenvalues of a graph is majorized by the conjugate sequence of its degrees allows to find easily general bounds for some Laplacian descriptors in terms of the conjugate sequence. We have shown here how to handle the conjugate sequence with a maximality argument, in order to express these bounds in terms of n and the average degree d_G , and with basic arguments for graphs with vertices of maximal or minimal degrees, in order to exhibit bounds given in terms of the number of these special vertices. We expect that in the future, as more relationships are uncovered for the conjugate sequence of the degrees of a graph, better bounds will be obtained in a similar way to those found here.

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Fractal–Like Kinetics Study of Adsorption on Multi–Walled Carbon Nanotube

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ABSTRACT

The fractal degree of adsorption on the carbon nanotube has been investigated. The fractal-like Langmuir kinetics model has been used to obtain the fractal degree of ion adsorption on carbon nanotube. The behavior of the fractal-like kinetics equation was compared with some famous rate equations like Langmuir, pseudo-first-order and pseudo-second-order equations. It is shown that the kinetic of adsorption onto carbon nanotube can be used to obtain its spectral dimension, successfully.

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1. INTRODUCTION

Physical, chemical and adsorption properties of adsorbents depend on its surface. The highly inhomogeneous surface structure of solid particles is difficult to characterize using simple geometry. Fractals, whose structures repeat themselves in all dimensions and on all length scales, are often used to depict the structure of solid particles and their surfaces. Adsorption is a method frequently used to determine the surface fractal dimension of porous media. It can be expected that adsorption processes involving solid–liquid interfaces could be of high heterogeneity.

The wide applicability of the fractal approach to adsorption systems and at the same time its limited utility in almost every case, brings one to the following conclusion: solid surfaces are never perfectly regular or irregular. Real solid surfaces represent an

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intermediate case. Several different theories have been developed to analyze adsorption data and obtain the surface fractal dimension [1, 2]. Avnir and Pfeifer [3] applied fractal geometry concepts to describe the general features of surface geometric heterogeneity in adsorption systems showing a small degree of surface organization. Ismail and Pfeifer [4] demonstrated three variants of the gas adsorption method for measurement of the surface fractal dimension, using carbon fibers as a test material. Ozek [5] provided methods to estimate pore and surface structures of activated carbon fiber by adsorption of dyes on the surface of and determined its fractal dimension. Lopez et al [6] presented a fractal kinetic model for adsorption at solid/solution interface.

2. PROBLEM STATEMENT

Carbon nanotube has brought on plenty of research in different scientific fields due to its special physical and chemical properties. The purpose of this study is to use this rate equation to analyze adsorption data of ions on some modified multi-walled carbon nanotubes. We are going to obtain the spectral dimension of some modified multi-walled carbon nanotubes by analysis of kinetic data.

3. PRELIMINARIES

There are famous kinetics model to describe rate of adsorption including pseudo-first-order, pseudo-second-order and Langmuir models. The Langmuir equation is the simplest adsorption isotherm with sound theoretical foundations that is considered a good approximation of the real adsorption systems. The Langmuir model is based on a kinetic principle. This model took into account the limited capacity of a flat and homogeneous surface as well as both adsorption and desorption processes [7]. The Langmuir rate equation is:

$$\frac{d\theta}{dt} = k_a\ c\,(1-\theta) - \ k_d\ \theta \tag{1}$$

where k_a is the adsorption rate coefficient, k_d is the desorption rate coefficient, $\theta = q/q_m$ is the relative surface coverage, q_m is the adsorption capacity and c is the concentration. By equating the rates of adsorption and desorption, the famous Langmuir isotherm will be obtained.

In 1998, Kopelman [8] considered that in most heterogeneous phases, the rate constant k_{obs} of reaction depends on reaction time:

$$k_{obs} = k'\,t^{-h} \qquad 0 \le h \le 1 \qquad (\mathrm{t} \ge 1) \tag{2}$$

where k' is a constant not dependent on time and h is a parameter measuring the degree of local heterogeneity [9]. When h=0, k_{obs} is time-independent; however, when $h \neq 0$, k_{obs} is time-dependent at all times.

The rate constant and the order of reaction are associated with the spectral dimension d_s. The spectral dimension d_s for fractal objects is a kind of dimension. It means the degree of local heterogeneity. Increase of d_s value implies more local heterogeneous, more remarkable time-dependent rate coefficient. For a single reactant bimolecular reaction (A+A), there should be the following relation:

$$h = 1 - \frac{d_s}{2} \tag{3}$$

The adsorption of the molecules on the active surface sites on can be written as:

$$\mathrm{B + mA \rightarrow B{-}mA} \tag{4}$$

where B is the adsorbate, A is the active site on surface and B−mA is the product of above reaction. Wang et al [10] developed the relations among the parameters of m, h and d_s to the adsorption kinetics of molecules onto fractal surfaces as:

$$d_s = 2\left(1 - \frac{h}{m}\right) \tag{5}$$

Recently, we developed a fractal-like kinetics equation for adsorption according to the Langmuir kinetic equation and fractal-like kinetics model [11]. This model studied the adsorption of some ions onto graphene surface, successfully.

4. PROPOSED METHOD

We proposed that rate coefficient of adsorption is time-dependent but rate coefficient of desorption is not [11]. This new rate equation is:

$$\frac{d\theta}{dt} = k_a t^{-h} c(1-\theta) - k_d \theta \tag{6}$$

The value of $k_a t^{-h}$ changes over time until equilibrium that the rate constant of adsorption reaches to $k_a^{'}$:

$$k_a^{'} = k_a t_e^{-h} \tag{7}$$

where t_e is the time in which system reaches to equilibrium. Therefore, the Langmuir constant (K_L) equals to:

$$K_L = \frac{k_a t_e^{-h}}{k_d} \tag{8}$$

The analytical solution of equation (6) led to a complex expression. One powerful technique for numerical simulations is stochastic simulation. For this purpose, we applied the CKS package developed by Houle and Hinsberg [12]. Recently, we have used it to solve some rate equations, numerically [13, 14].

In this method, the adsorption mechanism is considered as reaction (4). Since fractal-like Langmuir equation was used, the value of "m" in this reaction was considered equals to one. The input data for simulation are the rate constants, the value of h, and the initial concentrations of adsorbates in the bulk and the active sites on carbon nanotube. The rates of adsorption and desorption steps (R_i), are taken to be proportional to the probability, P_i, and calculated based on equation (6). The time step Δt between occurrences of any of the reaction steps is the mean time for a system obeying Poisson statistics:

$$\Delta t = \frac{-\ln \rho}{\sum R_i} \tag{9}$$

where ρ is a random number between 0 and 1. The simulation is propagated by repetitively selecting at random among the probability-weighted steps in the mechanism, and updating the reactant and product populations according to the stoichiometry of the selected step, system state variables, and reaction rates. The result is a set of concentration versus time curves that may be compared directly to experiment.

In the next section, this numerical solution method will be used to obtain the spectral dimension of multi-walled carbon nanotubes.

5. ILLUSTRATIVE EXAMPLES

In this section, the fractal-like Langmuir equation (equation (6)) will be used to determine the spectral dimension of multi-walled carbon nanotube. In addition, equation (6) will be compared with Langmuir kinetic model, pseudo-first-order and pseudo-second-order kinetic models. In order to determine the spectral dimension of multi-walled carbon nanotube, some experimental systems that have studied ion adsorption on the carbon nanotube were chosen [15, 16].

As an example, we have selected the system adsorption of Pb^{2+} on modified multi-walled carbon nanotube. Vukovic et al [15] studied Pb^{2+} ion adsorption on diethylenetriamine and triethylenetetramine modified multi-walled carbon nanotubes (e-MWCNT and d-MWCNT, respectively), experimentally. The experimental data were analyzed according to the Langmuir isotherm and the obtained values of K_L and q_m are shown in Table 1. Equilibrium data agree well with Langmuir isotherm. From the results, it is clearly seen that the equilibrium adsorption is much close to the experimental data, suggesting application of the kinetic Langmuir model. The curve fitting and statistical analyses were performed with CKS package. Having determined the parameters of Langmuir kinetic model, we used input data (temperature, concentration of adsorbent in solution and q_m) to fit the experimental kinetic plots by adjusting the value of the parameter k_a. The kinetic constants and correlation coefficient of this model were calculated and given in Table 2. Empirical (open diamond) and calculated data by kinetic Langmuir model (solid line) of Pb^{2+} ion adsorption on d-MWCNT are shown in Figure 1(a). As seen in Figure 1(a), the calculated data by kinetic Langmuir model are not in good agreement with empirical data.

Table 1: The initial concentration and Langmuir parameters for the adsorption of Pb^{2+} and Ni(II) onto modified multi-walled carbon nanotube.

Systems	c (mol/ℓ)	q_m (mg/g)	K_L (ℓ/mg)	R^2
Pb/d-MWCNT	2.40×10^{-5}	4.80×10^{1}	1.35	0.9879
Pb/e-MWCNT	2.40×10^{-5}	3.02×10^{1}	0.43	0.9885
Ni/MWCNT	1.00×10^{-3}	1.01×10^{1}	0.22	0.9879

The worse agreement between theory and experiment can be related to the fractal dimension of surface. Equation (6) was solved by CKS package and the values of k_a and h were obtained as adjustable parameters. The value of k_d was calculated by using equation (8). Figure 1(b) shows the agreement between theory and experiment, along with the values of the best-fit parameters (Table 2). There is noise in this fitting because of limited performance of the software. Figures 1(a) and 1(b) show the comparison of empirical kinetic data and calculated kinetic data fitted equations (1) and (6). A good fitting quality is obvious by equation (6) (see Table 2).

Table 2: The constant parameters of Langmuir and fractal-like Langmuir rate equations for the adsorption of Pb^{2+} and Ni(II) onto modified multi-walled carbon nanotube at 298 K.

Systems	Langmuir rate equation			Fractal-like Langmuir rate equation				
	k_a (ℓ/mol.min)	k_d (1/min)	R^2	k_a (ℓ/mol.min)	k_d (1/min)	h	d_s	R^2
Pb/d-MWCNT	4.00×10^{4}	0.14	0.9695	1.58×10^{4}	0.39×10^{-1}	0.67×10^{-1}	1.87	0.9899
Pb/e-MWCNT	2.70×10^{4}	0.30	0.9144	7.30×10^{3}	0.19×10^{-1}	0.28	1.44	0.9808
Ni/MWCNT	8.00×10^{2}	0.61×10^{-1}	0.9228	5.68×10^{2}	0.27×10^{-1}	0.10	1.80	0.9848

The pseudo-first-order and pseudo-second-order models are extensively used in the literatures. Azizian [17] showed that both pseudo-first- and pseudo-second-order equations are treated as special cases of Langmuir kinetic model. The pseudo-first-order equation is [18]:

$$\frac{dq}{dt} = k_1(q_e - q) \tag{10}$$

where k_1 is the pseudo-first-order rate coefficient.

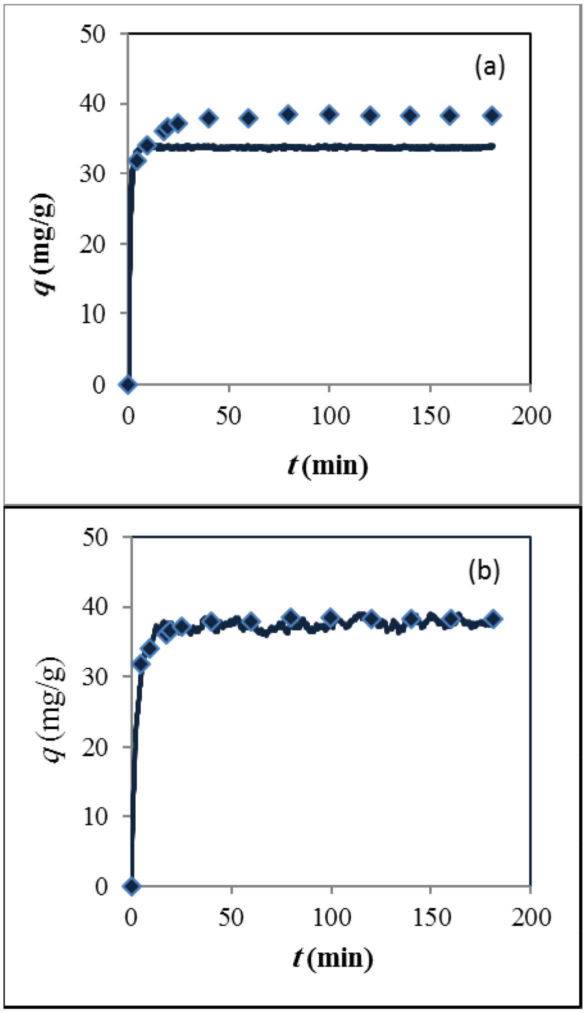

Figure 1. Kinetic data of Pb^{2+} adsorption on d-MWCNT surface; empirical [15] (diamonds) and calculated data (line) by a) Langmuir and b) the fractal-like Langmuir rate equations.

The pseudo-second-order kinetic equation is [19]:

$$\frac{dq}{dt} = k_2(q_e - q)^2 \tag{11}$$

where k_2 is the pseudo-second-order rate coefficient.

To compare equation (6) with pseudo-first-order and pseudo-second-order equations, empirical data of Pb^{2+} ion adsorption on d-MWCNT were fitted by them. Kinetic parameters along with correlation coefficients of the kinetic models are shown in Table 3. As can be seen from Tables 2 and 3, higher correlation coefficients (R^2) of equation (6) indicates that this kinetic model is suitable to describe adsorption of Pb^{2+} ion adsorption on d-MWCNT. Therefore, the fractal-like Langmuir equation was used to determine the spectral dimension of d-MWCNT and the result was shown in Table 2.

Table 3: The pseudo-first-order and pseudo-second-order parameters for the adsorption of Pb^{2+} and Ni(II) onto modified multi-walled carbon nanotube at 298 K.

Systems	Pseudo-first-order		Pseudo-second-order		
	k_1(1/min)	R^2	q_e(mg/g)	k_2(g/mg.min)	R^2
Pb/d-MWCNT	7.92×10^{-2}	0.8400	3.88×10^{1}	4.04×10^{-2}	0.9675
Pb/e-MWCNT	7.48×10^{-2}	0.9053	2.87×10^{1}	1.35×10^{-2}	0.9775
Ni/MWCNT	1.80×10^{-1}	0.9362	5.14	2.98×10^{-2}	0.9291

Now let us consider the experimental data of Pb^{2+} ion adsorption on e-MWCNT. For this purpose, we have applied the procedure described in the previous sections. The results of that fitting are shown in Figures 2(a) and 2(b) (solid lines), whereas the related best-fit parameters are collected in Table 2. When looking through Figures 2(a) and 2(b) one can state that equation (6) offers a better fit of kinetic data than kinetic Langmuir model.

A comparison of the kinetic models and the empirical kinetic data of Pb^{2+} ion adsorption on e-MWCNT was best described by equation (6). The obtained parameters of kinetic models are presented in Table 3. It was found that equation (6) is superior to other three ones for the description of kinetic data. Thus, the fractal-like Langmuir equation was used to determine the spectral dimension of e-MWCNT (Table 2).

In continuous, another experimental system was studied. This empirical system was presented by Chen et al [16] has studied Ni(II) adsorption on a kind of modified multi-walled carbon nanotube. In the first step, we fitted the empirical kinetic data by using equations (1) and (6) (Tables 2 and 3). The calculated data by equation (1) are shown in Figure 3(a). Figure 3(b) shows that equation (6) can correlate very well the behavior Ni(II) adsorption on modified multi-walled carbon nanotube. By looking at Figures 3(a) and 3(b), we observe a good suitability of equation (6) rather the kinetic Langmuir equation.

Finally, empirical data Ni(II) adsorption on modified multi-walled carbon nanotube were studied by pseudo-first-order and pseudo-second-order equations. The estimated model parameters with the correlation coefficient (R^2) for the different models are shown in Table 3. The correlation coefficients, R^2, given in the Tables 2 and 3 also show that equation (6) can be satisfactorily described empirical data of Ni(II) adsorption on a modified multi-walled carbon nanotube. The obtained value of spectral dimension of modified multi-walled carbon nanotube was shown in Table 2.

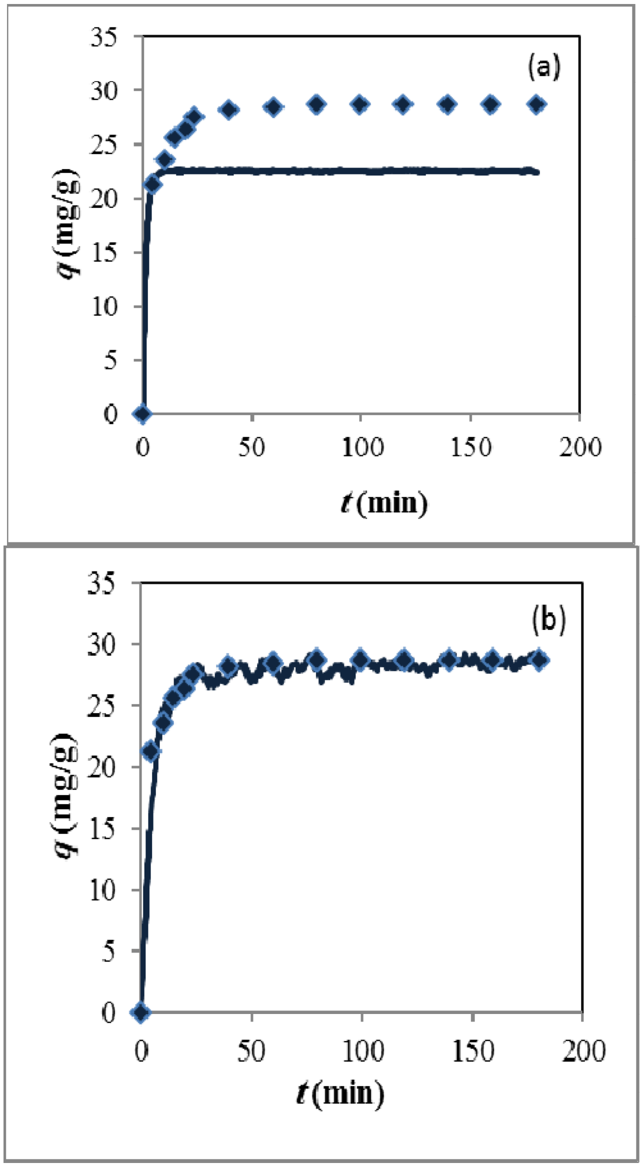

Figure 2. Kinetic data of Pb^{2+} adsorption on e-MWCNT surface; empirical [15] (diamonds) and calculated data (line) by a) Langmuir and b) the fractal-like Langmuir rate equations.

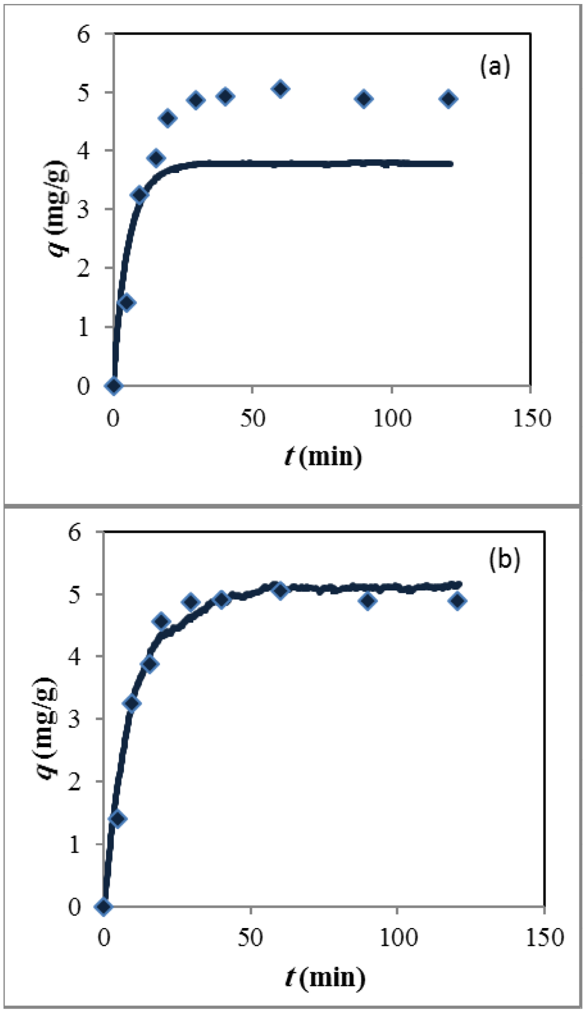

Figure 3. Kinetic data of Ni(II) adsorption on MWCNT surface; empirical [16] (diamonds) and calculated data (line) by a) Langmuir and b) the fractal-like Langmuir rate equations.

In summary, the presented model investigation seems to suggest that equation (6) is a very good equation to correlate kinetic data of adsorption on carbon nanotube surfaces and can be used to obtain the spectral dimension of surfaces.

6. CONCLUSION

By applying empirical data of Pd(II) and Ni(II) adsorption on carbon nanotube surfaces, it was shown that the fractal-like Langmuir model can be applied with good success in many adsorption systems. The best description of kinetics was obtained with the fractal-like Langmuir equation corresponding to Langmuir, pseudo-first-order and pseudo-second-order rate equations. By using of empirical data of ion adsorption on multi-walled carbon nanotube, the fractal degree of adsorption (h) was obtained. The spectral dimensions of some multi-walled carbon nanotubes were obtained.

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On Common Neighborhood Graphs II

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ABSTRACT

Let G be a simple graph with vertex set $V(G)$. The common neighborhood graph or congraph of G, denoted by $con(G)$, is a graph with vertex set $V(G)$, in which two vertices are adjacent if and only if they have at least one common neighbor in G. We compute the congraphs of some composite graphs. Using these results, the congraphs of several special graphs are determined.

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1 INTRODUCTION AND PRELIMINARIES

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For any vertex $v \in V(G)$, the set of neighbors of v is the set $N_v(G) = \{u \in V(G) | \, uv \in E(G)\}$. We say that $v \in V(G)$ is an isolated vertex if $N_G(v)$ is an empty set. The distance between the vertices u and v of G denoted by $d_G(u,v)$. ($d(u,v)$for short), is defined as the length of the shortest path connecting u and v.

The complement of a graph G is a graph H on the same vertices such that two vertices of H are adjacent if and only if they are not adjacent in G. The graph H is usually denoted by $\bar{G}$.The minimum length of a cycle in a graph G is called the girth of G. We

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now define several kinds of products of pairs of graphs; see [14] for details.The union of the simple graphs G and H is the graph $G \cup H$ with vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$. If G and H are disjoint, then we refer to their union as a disjoint union. Suppose that G and H are two graphs with disjoint vertex sets. Their Cartesian product $G \times H$ is a graph such that $V(G \times H) = V(G) \times V(H)$, and two vertices (u_1, v_1) and (u_2, v_2) are adjacent in $G \times H$ if and only if either $u_1 = u_2$ and v_1 is adjacent with v_2, or $v_1 = v_2$ and u_1 is adjacent with u_2. The join $G + H$ of the graphs G and H is the graph union $G \cup H$ together with all the edges joining $V(G)$ and $V(H)$. The tensor product $G \otimes H$ of the graphs G and H is the graph with vertex set $V(G) \times V(H)$ in which (u_1, v_1) is adjacent with (u_2, v_2) whenever $u_1u_2 \in E(G)$ and $v_1v_2 \in E(H)$. The strong product $G\Omega H$ of G and H has the vertex set $V(G\Omega H) = V(G) \times V(H)$ and two distinct vertices (u_1,v_1) and (u_2,v_2) of $G\Omega H$ are adjacent if $u_1 = u_2$ and $v_1v_2 \in E(G)$., or $u_1u_2 \in E(G)$ and $v_1 = v_2$, or $u_1u_2 \in E(G)$ and $v_1v_2 \in E(H)$.. For given vertices $y \in V(G)$ and $z \in V(H)$, a splice of G and H by vertices y and z, $(G.H)(y,z)$, is defined by identifying the vertices y and z in the union of G and H [10]. Hou and Shiu [13] introduced an edge version of corona product as follows.

Let G and H be two graphs on disjoint sets of n_1,n_2 vertices and m_1, m_2 edges, respectively. The edge corona $G \lozenge H$ is defined as the graph obtained by taking one copy of G and m_1 copies of H, then joining two end-vertices of the i-th edge of G to every vertex in the i-th copy of H.

Now, we define the Hajós join which is introduced in [11]. Let G and H be two graphs, $vw \in E(G)$, and $xy \in E(H)$. Then the Hajós join of these two graphs, which is denoted by $G\Delta H$,is a new graph that combines the two graphs by identifying vertices v and x into a single vertex, removing the two edges vw and xy, and adding a new edge wy. For example, if G and H are cycles of length p and q respectively, then the Hajós join of these two cycles is itself a cycle, of length $p + q - 1$.

Let G be a simple graph with vertex set $\{v_1, v_2, \dots, v_n\}$. The common neighborhood graph (congraph) of G, denoted by $con(G)$, is a graph with the vertex set $\{v_1, v_2, \dots, v_n\}$. in which two vertices are adjacent if and only if they have at least one common neighbor in the graph G [1, 2].

Congraphs have been investigated in several earlier works [1, 2, 6, 12, 15]. In [12], we obtained some results on congraphs of graph products. In this paper we continue this study and report additional results along these lines.

It should be noted that in two earlier works [3, 4] the so-called derived graph $G^\dagger$ of the graph G was considered. The derived graph $G^\dagger$ has the same vertex set as the parent graph G, and two vertices of $G^\dagger$ are adjacent if and only if their distance in G is equal to

two. It is immediately seen that $G^{\dagger} = con(G)$ if and only if the parent graph G does not contain triangles. Thus, in particular, $G^{\dagger} = con(G)$ holds whenever G is bipartite.
The notations used in this paper is standard and taken mainly from [5, 14]. In what follows, the graphs considered are assumed to be simple. If a graph has parallel edges, we consider these as a single edge.

2 COMMON NEIGHBORHOOD GRAPHS OF SOME GRAPH OPERATIONS

In this section we obtain $con(G)$ for some operations on two graphs. We begin with the tensor product. To do this, we state the following lemma which immediately follows from the definition of the operation $\otimes$.

Lemma 2.1. Let (v_i, u_j) and (v_r, u_s) be two vertices of $G \otimes H$. Then $(v_k, u_t) \in N_{G\otimes H}(v_i, u_j) \cap N_{G\otimes H}(v_r, u_s)$ if and only if $v_k \in N_G(v_i) \cap N_G(v_r)$ and $u_t \in N_H(u_j) \cap N_H(u_s)$.

Theorem 2.2. Let G and H be two graphs without isolated vertices. Then

$$con(G \otimes H) = con(G) \Omega \, con(H).$$

Proof. Let (v_i, u_j) and (v_r, u_s) be two vertices of $G \otimes H$ such that $v_i \neq v_r$ and $u_j \neq u_s$. If $(v_i, u_j)(v_r, u_s)$ is an edge of $con(G \otimes H)$, then there is a vertex $(v_k, u_t) \in V(G \otimes H)$ such that $(v_k, u_t) \in N_{G\otimes H}(v_i, u_j) \cap N_{G\otimes H}(v_r, u_s$So by Lemma 2.1, $v_k \in N_G(v_i) \cap N_G(v_r)$ and $u_t \in N_H(u_j) \cap N_H(u_s)$. Therefore $v_i v_r \in E(con(G))$ and $u_j u_s \in E(con(H))$. This means that for $v_i \neq v_r$ and $u_j \neq u_s$it holds that $(v_i, u_j)(v_r, u_s)$ is an edge of $con(G \otimes H)$ if and only if $v_i v_r \in E(con(G))$ and $u_j u_s \in E(con(H))$..

Assume that $v_i = v_r = v$. If $(v, u_j)(v, u_s)$ is an edge of $con(G \otimes H)$, then there is a vertex (v_k, u_t) such that $(v_k, u_t) \in N_{G\otimes H}(v, u_j) \cap N_{G\otimes H}(v, u_s)$. By Lemma 2.1, we have $v_k \in N_G(v)$ and $u_t \in N_H(u_j) \cap N_H(u_s)$. So if $v_i = v_r$, then $u_j u_s \in E(con(H))$. Therefore, for $v_i = v_r$ it holds that $(v_i, u_j)(v_r, u_s)$ is an edge of $con(G \otimes H)$ if and only if $v_i = v_r$ and $u_j u_s \in E(con(H))$. Similarly if $u_j = u_s$, then $(v_i, u_j)(v_r, u_s)$ is an edge of $con(G \otimes H)$ if and only if $u_j = u_s$ and $v_i v_r \in E(con(G))$.

Hence $con(G \otimes H) = (con(G) \otimes con(H)) \cup (con(G) \times con(H)) = con(G) \, \Omega \, con(H)$ and this completes the proof. ■

In the following theorem, we determine the congraph of Hajós join.

Theorem 2.3. Let G and H be two graphs with the girth at least 5. Then

$$\begin{aligned} con(G\Delta H) &= (con(G)\cdot con(H))(v,x) - E(y+N_H(x)) - E(w+N_G(v)) - E(x+N_H(y)) \\ &\quad - E(v+N_G(w)) \cup E((N_G(v)-\{w\})+(N_H(x)-\{y\})) \cup E(N_G(w)+y) \\ &\quad \cup E(N_H(y)+w), \end{aligned}$$

where for two vertices r, s, the notation $E(r + N(s))$ denotes the edges of the join of the vertex r and the neighbors of s.

Proof. In the structure of Hajós join, if we don't remove two edges vw and xy, and don't add a new edge wy, we can arrive to splice of two graphs G and H. So we consider the graph $\big(con(G).con(H)\big)(v,x)$ as the base of the common neighborhood graph of the Hajós join of G and H. Then we investigate the effect of removing the two edges vw and xy, and adding a new edge wy.

Since the girth of the graph G is at least 5, when we remove the edge vw, all the edges wr and vs in $con(G)$, $r \in N_G(v)$ and $s \in N_G(w)$, that have v and w as the common neighbor, respectively, will be deleted. Similarly when we eliminate the edge xy, all the edges ya and xb in $con(H)$, $a \in N_H(x)$ and $b \in N_H(y)$, that have x and y as the common neighbor, respectively, will be deleted. Continuing this argument, when we identify the vertices v and x into a single vertex, then $N_G(v) - w$ and $N_H(x) - y$ will have a common neighbor. So each vertex in $N_G(v) - w$ will be adjacent to each vertex in $N_H(x) - y$. By adding the new edge wy, w will become the common neighbor between y and $N_G(w)$ and y the common neighbor between w and $N_H(y)$. ■

Applying the Hajós join to two copies of K_4 by identifying a vertex from each copy into a single vertex, deleting an edge incident to the combined vertex within each subgraph, and adding a new edge connecting the endpoints of the deleted edges, produces the Moser spindle, see Fig. 1. As an application we characterize the common neighborhood graph of the Moser spindle.

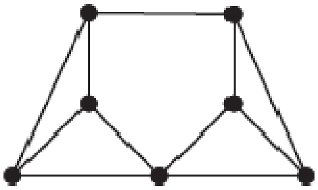

Figure 1. The Moser Spindle Graph.

Corollary 2.4. The common neighborhood graph of the Moser spindle is $K_7 - e$.

In the next theorem, we compute the common neighborhood graph of the edge corona product of graphs. One can see that the edge corona product of G with a complete graph K_t, and the common neighborhood graph of G are subgraphs of $G \lozenge H$.

Theorem 2.5. Let G be a graph with n vertices and m edges and H be a graph with t vertices. Then

$$con(G\lozenge H) = (G\lozenge K_t) \cup con(G) \cup \left(\bigcup_{e_k=v_iv_j} \big(N_G(v_i) \cup N_G(v_j)\big) + H_k\right)$$
$$\cup \left(\bigcup_{e_i=v_lv_q, e_j=v_lv_{q'}} (H_i + H_j)\right).$$

Proof. Let $V = \{v_1, \dots, v_n\}$, $E(G) = \{e_1, \dots, e_m\}$, and $V(H) = \{u_1, \dots, u_t\}$. Denote the i-th copy of H in $G \lozenge H$, by H_i. Each two vertices of H_i have the end vertices of e_i as common neighbors, So the induced subgraph of $con(G \lozenge H)$ on each H_i is a complete graph. On the other hand, a vertex in H_i has a common neighbor with a vertex in H_j if and only if the edges e_i and e_j are adjacent. So the induced subgraph of $G \lozenge H$ on the vertices $H_i \cup H_j$ is $H_i + H_j$ if and only if e_i and e_j are adjacent in G and there is no edge between H_i and H_j if e_i and e_j are not adjacent in G.

We now consider the vertices $\{v_1, \dots, v_n\}$. Clearly, v_i and v_j have a common neighbor v_k in $G \lozenge H$ if and only if v_k is their common neighbor in G. Also v_i and v_j have a common neighbor u_r in $G \lozenge H$, if and only if $v_i v_j$ is an edge of G.

Finally, a vertex v_s in G has a common neighbor with a vertex u_r in H_k if and only if v_s is in $N_G(v_i) \cup N_G(v_j)$, where $e_k = v_i v_j$. This completes the proof. ■

By definition, the edge corona $T \lozenge S_n$ of a tree T of order n and S_n is the graph obtained by taking one copy of T and $n-1$ copies of S_n and then joining two end-vertices of the i-th edge of T to every vertex in the i-th copy of S_n.

Corollary 2.6. The common neighborhood graph of the edge corona product of graphs K_2 and S_n satisfies $con(K_2 \lozenge S_n) = K_{n+2}$.

3. RELATION BETWEEN SOME SPECIAL GRAPHS AND THEIR CONGRAPHS

In this section we compute the common neighborhood graphs of the central graph, line graph, shadow graph, and Mycielski graph.So we should first define these graphs.

For a given graph G, the line graph of G is denoted by $L(G)$ and the vertices of $L(G)$ are the edges of G. Two edges of G that share a vertex are considered to be adjacent in $L(G)$. The subdivision graph of the graph G is denoted by $S(G)$ and is the graph obtained by inserting an additional vertex in each edge of G. Equivalently, each edge of G is replaced by a path of length 2.

For a given graph G, we do an operation on G by subdividing each edge exactly once and joining each pair of vertices of the original graph which were previously non-adjacent. The graph obtained by this process is said to be the central graph of G, denoted by $C(G)$, [17, 18, 19].

The shadow graph $D_2(G)$ of a connected graph G is constructed by taking two copies of G say G' and G'' and joining each vertex u' in G' to the neighbors of the corresponding vertex u'' in G''. For example, $D_2(C_4)$ is depicted in Fig. 2.

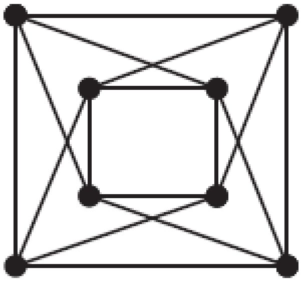

Figure 2. The Shadow Graph $D_2(C_4)$.

The Mycielski graph of G was introduced by J. Mycielski [16] for the purpose of constructing triangle–free graphs with arbitrarily large chromatic number. This graph has been much studied [7, 8, 9].

Let G be a graph with vertex set $\{v_1, v_2, \dots, v_n\}$. The Mycielski graph $\mu(G)$ of G contains G itself as an isomorphic subgraph, together with $n + 1$ additional vertices: a vertex $u_i$which corresponds to each vertex v_i of G, and another vertex w. Each vertex u_i is connected by an edge to w, so that these vertices form a subgraph in the form of a star $K_{1,n}$. In addition, for each edge v_iv_j of G, the Mycielski graph includes two edges, u_iv_j and v_iu_j. In Fig. 3 we shows Mycielski's construction applied to a 5-vertex cycle. The resulting Mycielskian is the Grötzsch graph, an 11-vertex graph with 20 edges. The Grötzsch graph is the smallest triangle–free 4-chromatic graph.

Theorem 3.1. Let G be a graph. Then

$$con(C(G)) = G \cup L(G) \cup con(\overline{G}) \cup \left(\bigcup_{e=uv\in E(G)} [v_e + (V(G) - (N_G(u) \cup N_G(v)))]\right).$$

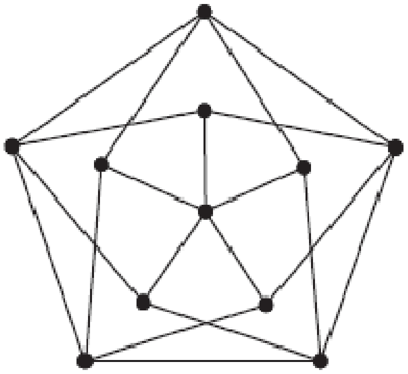

Figure 3. The Grötzsch Graph.

Proof. Let $V(G) = \{v_1, \dots, v_n\}$ and $E(G) = \{e_1, \dots, e_m\}$. So the set of vertices of $C(G)$ is $V(C(G)) = \{v_1, \dots, v_n, v_{e_1}, \dots, V_{e_m}\}$, where v_{e_i} is the vertex inserted in the edge e_i, $(1 \leq i \leq m)$. We determine the graph $con(C(G))$ in three steps:

(i) We find the edges between the vertices of $\{v_1, v_2 \dots, v_n\}$. The vertices v_i and v_j have a common neighbor in the set $\{v_{e_1}, \dots, V_{e_m}\}$, of graph $C(G)$ if and only if $v_i v_j$ is an edge in the graph G. Also the vertices v_i and v_j have a common neighbor in the set $\{v_1, \dots, v_n\}$ of the graph $C(G)$ if and only if v_i and v_j have a common neighbor in the graph $\bar{G}$. So the subgraph induced by the vertices $v_1, \dots, v_n$ in the graph $C(G)$ is $G \cup con(\bar{G})$.

(ii) We consider the subgraph of $C(G)$ induced by the set $\{v_{e_1}, \dots, V_{e_m}\}$,. It is easy to see that v_{e_i} and v_{e_j} do not have common neighbors in $\{v_{e_1}, \dots, V_{e_m}\}$,. On the other hand, v_{e_i} and v_{e_j} have the vertex v_t as common neighbor in $\{v_1, v_2 \dots, v_n\}$. if and only if the edges e_i and e_j have the vertex v_t as the common vertex in G. Therefore the respective induced subgraph is $L(G)$.

(iii) We find the edges between $\{v_1, v_2, \dots, v_n\}$ and $\{v_{e_1}, \dots, v_{e_m}\}$. Let $e_i = v_r v_s$ be an edge of G. So $N_{C(G)}(v_{e_i}) = \{v_r, v_s\}$ and this means that v_{e_i} is adjacent in $con(C(G))$ to the vertices that are neighbors of v_r and v_s. By the definition of $C(G)$, the edges between $\{v_1, v_2, \dots, v_n\}$ and $\{v_{e_1}, \dots, v_{e_m}\}$ are $\bigcup_{e=uv \in E(G)} [v_e + \big(V(G) - (N_G(u) \cup N_G(v))\big)]$.
Combining (i), (ii), and (iii), the theorem follows. ■

In the graph G, let $\{e_1, \dots, e_k\}$ be all of the edges incident to vertex u. We denote the set of $\{v_{e_1}, \dots, v_{e_k}\}$ in the graph $L(G)$ by $N_G(u)$. That v_{e_i} is a vertex of $L(G)$ corresponding to an edge e_i of G.

Theorem 3.2. Let G be a graph. Then $con(L(G)) = \bigcup_{e=uv\in E(G)} (N'_G(u) + N'_G(v))$.

Proof. Consider the vertices $\{v_{e_1}, \ldots, v_{e_m}\}$ in $L(G)$. If $e_i = v_r v_s$ is an edge in G, then v_{e_i} can be as the common neighbor of the sets $N'_G(v_r)$ and $N'_G(v_s)$. So for each $e_i = v_r v_s$ in G, $N'_G(v_r) + N'_G(v_s)$ is the subgraph of $con(L(G))$. ■

Theorem 3.3. Let G be a graph without isolated vertices and G' and G'' be two copies of G. Then $con(D_2(G)) = D_2(con(G)) \bigcup \{v'_i v''_i \mid v'_i \in V(G'), v''_i \in V(G''), 1 \le i \le |V(G)|\}$.

Proof. Suppose that $V(G) = \{v_1, v_2, \ldots, v_n\}$, $V(G') = \{v'_1, v'_2, \ldots, v'_n\}$, and $V(G'') = \{v''_1, v''_2, \ldots, v''_n\}$,. By definition of the shadow graph, it is easy to see that $v'_t \in N_{G'}(v'_r) \cap N_{G'}(v'_s)$ if and only if $v''_t \in N_{G'}(v'_r) \cap N_{G'}(v'_s)$. Similarly, $v''_t \in N_{G'}(v''_r) \cap N_{G'}(v''_s)$ if and only if $v''_t \in N_{G'}(v'_r) \cap N_{G'}(v'_s)$. Therefore, the subgraph of $con(D_2(G))$ induced on $V(G')$ is $con(G')$ and induced on $V(G'')$ is $con(G'')$. ■

We now determine the edges between $V(G')$ and $V(G'')$. To do this, for two vertices v_i and v_j, $i \neq j$, we use the following facts resulting from the definition of shadow graph:

1) $v'_k \in N_{G'}(v'_i) \bigcap N_{G''}(v''_j)$ if and only if $v''_k \in N_{G'}(v'_i) \bigcap N_{G''}(v''_j)$.

2) $v'_k \in N_{G'}(v'_i) \bigcap N_{G'}(v'_j)$ if and only if $v'_k \in N_{G'}(v'_i) \cap N_{G''}(v''_j)$.

Therefore, uv is an edge of $con(G)$ if and only if $u'v''$ and $v'u''$ are edges of $con(D_2(G))$. On the other hand, since G has no isolated vertices, for each i, $1 \le i \le |V(G)|$, $v'_i v''_i$ are edges of $con(D_2(G))$. and the proof is completed. ■

Corollary 3.4. For path P_n and complete graph K_2 the following equality holds:

$$con(D_2(P_n)) = con(P_n) \times K_2 .$$

Theorem 3.5. Let G be a graph with n vertices. Then the congraph of its Mycielski graph contains $con(G)$ as an isomorphic subgraph, together with $n + 1$ additional vertices: a vertex u_i corresponding to each vertex v_i of $con(G)$ such that the induced graph of $\mu(G)$ on them is K_n and another vertex w. Each vertex v_i is connected by an edge to w, so that these vertices form a subgraph in the form of a star $K_{1,n}$. In addition, for each edge $v_i v_j$ of $con(G)$, the common neighborhood graph of the Mycielski graph includes two edges,$u_i v_j$ and $v_i u_j$.

Proof. Since in the Mycielski graph, each vertex u_i is connected by an edge to w, so vertex w is the common neighborhood of vertices $u_1, \dots, u_n$ in the graph $\mu(G)$ and this implies that the subgraph of $\mu(G)$ induced on these vertices is K_n . It is clear that $v_t \in N_{\mu(G)}(v_r) \cap N_{\mu(G)}(v_s)$ if and only if $u_t \in N_{\mu(G)}(v_r) \cap N_{\mu(G)}(v_s)$, so the subgraph of $\mu(G)$ induced on $\{v_1, \dots, v_n\}$ is $con(G)$. Also by the definition of Mycielski graph, since G has not isolated vertices, the vertices u_i are common neighborhoods of the vertices v_j and w. This implies that,$v_i w \, 1 \le i \le m$are edges of $con(\mu(G)$).

Now we obtain the edges between $\{v_1, \dots, v_n\}$ and $\{u_1, \dots, u_n\}$. Let the vertex v_k be the common neighbor of the vertices v_i and v_j. By the definition of Mycielski graph, we have the following cases:

Case 1. The vertex v_k is in the common neighborhood of vertices v_j and u_j in graph G. This implies that $v_j u_j$, $1 \le j \le m$are edges of the congraph.

Case 2. The vertex v_k is in the common neighborhood of the vertices v_j and u_i, v_i and u_j in graph G. This implies that for each edge $v_i v_j$ of $con(G)$, the common neighborhood graph of $\mu(G)$ includes two edges $u_i v_j$ and $v_i u_j$ and this completes the proof. ■

As an application we compute the common neighborhood graph of Grötzsch graph.

Corollary 3.6. Let $C_5 : v_1 v_2 v_3 v_4 v_5 v_1$. Then the common neighborhood graph of the Grötzsch graph is determined via $(w + C_5) \cup K_5 \cup \{v_i u_{i+1} \mid 1 \le i \le 4\} \cup \{v_{i+1} u_i \mid 1 \le i \le 4\} \cup v_1 u_5 \cup v_5 u_1$.

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On the Eccentric Connectivity Index of Unicyclic Graphs

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ABSTRACT

In this paper, we obtain the upper and lower bounds on the eccentricity connectivity index of unicyclic graphs with perfect matchings. Also we give some lower bounds on the eccentric connectivity index of unicyclic graphs with given matching numbers.

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1 INTRODUCTION

Throughout this paper, G will denote a simple connected graph with n vertices (labeled by $v_1, v_2, ..., v_n$). Moreover, for $1 \le i \le n$, the neighbor and the degree of each vertex v_i will be denoted by $N(v_i)$ and d_{v_i}, respectively. For two vertices u and v in $V(G)$, we denote by $d(u,v)$ the distance between u and v i.e. the length of the shortest $u-v$ path in G.

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A pendant vertex is a vertex of degree 1 and a pendant edge is an edge incident to a pendant vertex. Denote by PV the set of pendant vertices of a graph G.

The eccentricity of a vertex u in a graph G, denoted by e_u, is the maximum distance from u to any vertex. That is, $e_u = \max\{d(u,v) : v \in V\}$.

A matching M of a graph G is a subset of $E(G)$ such that no two edges in M share a common vertex. The matching number of G, denoted by m, is the number of edges of a maximum matching in G. If every vertex of G incident with an edge of M, then the matching M is perfect.

Denote by C_n the cycle on n vertices. A unicyclic graph is a connected graph with a unique cycle. Other undefined terminologies and notations of graphs may refer to [2].

Molecular descriptors have found a wide application in QSPR / QSAR studies [15]. Among them, topological indices have a prominent place.

Sharma, Goswami and Madan [14] introduced a distance-based topological index which named eccentric connectivity index $\xi^c(G)$ as follows:

$$\xi^c(G) = \sum_{u \in V(G)} d_u e_u .$$

The eccentric connectivity index has been employed successfully for the development of numerous mathematical models of biological activities of diverse nature [7,8,13,14].

Recently Ashrafi et. al. [1] obtained exact formulas for the eccentric connectivity index of $\mathrm{TUC_4C_8(s)}$ nanotube and $\mathrm{TC_4C_8(s)}$ nanotorus. Ilič and Gutman [6] examined the eccentric connectivity index of chemical trees. In [18], Zhou et al. gave mathematical properties of eccentric connectivity index. Also in [11], the authors investigated the eccentric connectivity index of trees. Moreover, in [17], Zhang investigated the eccentric connectivity index of unicyclic graphs. Recall that in mathematical chemistry a unicyclic graph with perfect matching is known as conjugated unicyclic graphs. We may refer [9,10] for more and some other details on conjugated unicyclic graphs.

In this paper, we present upper and lower bounds on the eccentric connectivity index of unicyclic graphs with perfect matchings. Also we give lower bounds on the eccentric connectivity index of unicyclic graphs with given matching numbers.

Throughout this paper, U_n denote unicyclic graphs with n vertices and $U(n,m)$ denote unicyclic graphs with n vertices and m matchings. Let $U(2m,m)$ be the set of unicyclic graphs with perfect matching and $2m$ vertices. We make use of the following results in this paper.

Lemma 1.1. [3] *Let* $G \in U(2m,m)$, *where* $m \geq 3$, *and let T be a branch of* G *with the root* r. *If* $u \in V(T)$ *is a pendant vertex furthest from the root* r *with* $d_G(u,r) \geq 2$, *then u is adjacent to a vertex v of degree two.*

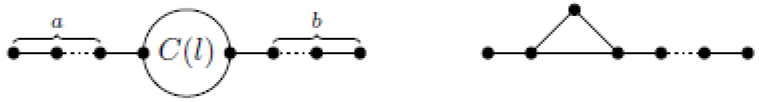
Lemma 1.2. [12] *Let* $G \in U(2m,m)$. *If* $PV \neq \emptyset$, *then for any vertex* $u \in V(G)$, $|N(u) \cap PV| \leq 1$.

Lemma 1.3. [16] *Let G be a graph in* $U(n,m)$ *and* $G \circledR C_n$, *where* $(n > 2m)$. *Then there is an* $m-$*matching M and a pendant vertex v such that M does not saturate v.*

Theorem 1.4. [6] *Let* w *be a vertex of a nontrivial connected graph G. For non-negative integers p and q, let G(p,q) denote the graph obtained from G by attaching to the vertex w pendent paths* $P = wv_1v_2...v_p$ *and* $Q = wu_1u_2...u_q$ *of lengths p and q, respectively. If* $p \geq q \geq 1$, *then*

$$\xi^c(G(p,q)) = \xi^c(G(p+1,q-1)).$$

Let P_n^3 denote the unicyclic graph obtained from C_3 by identifying one of its vertices with a pendant vertex of the path P_{n-2}. Let $C_{a,b}(l)$ denote the unicyclic graph obtained from $C(l)$ by attaching the path P_a at one vertex and the path P_b at another vertex. Let $C_{a,b}(l)$ and N_n^3 denote unicyclic graphs of the forms as depicted in Figure 1.



$C_{a,b}(l)$ where $a, b \geq 1$ N_n^3

Figure 1

Lemma 1.5. [17] *Let G be a graph in* U_n *with* $n \geq 5$ *vertices. If* $G \in C_{a,b}(l)$ *and* $G \circledR N_n^3$, *then* $\xi^c(P_n^3) > \xi^c(N_n^3) > \xi^c(G)$.

Theorem 1.6. [17] *Let G be a graph in* U_n, $n \geq 5$. *Then*

$$\xi^c(G) \leq \xi^c(P_n^3) = \begin{cases} \frac{1}{2}(3n^2 - 4n - 6)\ , & n \text{ is even} \\ \frac{1}{2}(3n^2 - 4n - 5)\ , & n \text{ is odd}, \end{cases}$$

where the equality holds if and only if $G \circledR P_n^3$.

2 MAIN RESULTS

After all above material, we are ready to present our results on the bounds for the eccentric connectivity index of unicyclic graphs. Let H_1^m be the graph on $2m$ vertices obtained from C_3 by attaching a pendant edge together with $m-2$ paths of length 2 at one vertex. Let H_2^m be the graph on $2m$ vertices obtained from C_3 by attaching a pendant edge and $m-3$ paths of length 2 at one vertex, and single pendant edges at the other vertices. Let H_3^m be the graph on $2m$ vertices obtained from C_3 by attaching a pendant edge at one vertex and $m-2$ paths of length 2 at another vertex. Let H_4^m be the graph on $2m$ vertices obtained from C_4 by attaching $m-2$ paths of length 2 at one vertex.

Let H_5^m be the graph on $2m$ vertices obtained from C_4 by attaching a pendant edge atone vertex and $m-3$ paths of length 2 at another vertex. H_1^m, H_2^m, H_3^m, H_4^m and H_5^m are shown in Figure 2.

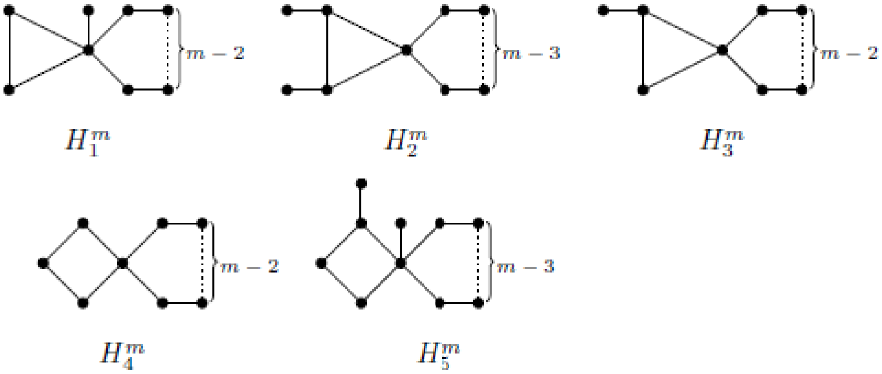


Figure 2

Theorem 2.1. *Let* $G \in U(2m,m)\setminus\{H_1^m, H_2^m, H_3^m\}$, *where* $m \geq 5$. *Then* $\xi^c(G) \geq 12m$. *The equality holds if and only if* $G \cong H_4^m$ *or* $G \cong H_5^m$.

Proof. We prove the result by induction on m. By direct calculation, we see that the result is provided for $m=5$. Let $m \geq 5$. We assume that the result holds for graphs in $U(2m-2, m-1)$.

Case 1. G has a pendant vertex u which is adjacent to a vertex v of degree two. Let w be adjacent of v different from u. In this case, $uv \in M$. Let $G' = G-u-v$. Then $G' \in U(2m-2, m-1)$. Obviously, if $e_u = e$, then $e_v = e-1$ and $e_w = e-2$ since $m \geq 5$. Also since $m \geq 5,\ e \geq 4$. We know that $e_t = e_t^{'}$ or $e_t = e_t^{'} + 1$ or $e_t = e_t^{'} + 2$ for $t \in V(G) - \{u, v, w\}$. Therefore, we write

$$\xi^c(G) - \xi^c(G^{'}) = e_u d_u + e_v d_v + e_w d_w - e_{w^{'}} d_{w^{'}} + \sum_{t \in V(G) - \{u,v,w\}} d_t \left[e_t - e_t^{'} \right]$$

$$= e.1 + 2(e-1) + d_w(e-2) - (d_w - 1)(e-2) + \sum_{t \in V(G) - \{u,v,w\}} d_t \left[e_t - e_t^{'} \right]$$

$$= 4e - 4 + \sum_{t \in V(G) - \{u,v,w\}} d_t \left[e_t - e_t^{'} \right]. \qquad (1)$$

Using the equality (1), we get the following inequality $\xi^c(G) \geq \xi^c(G^{'}) + 4e - 4$. Using the induction hypothesis and the fact $e \geq 4$, we have $\xi^c(G) \geq 12(m-1) + 4.4 - 4 = 12m$. This is the required result.

Case 2. G is a cycle C_k together with some pendant edges attached to some vertices on C_k. If $G \cong C_{2m}$ then $\xi(G) = 4m^2 \geq 12m$ for $m \geq 5$. Let $G \circledR C_{2m}$. Let p and q denote the number of pendant vertices and the number of vertices with degree two in G, respectively. Therefore, the number of vertices with degree three be p. Note that we have $2p + q = 2m$ and $p \leq m$. Let $V_1(G) = \{u \in V(G) : d_u = 1\}$, $V_2(G) = \{v \in V(G) : d_v = 2\}$ and $V_3(G) = \{t \in V(G) : d_t = 3\}$. If u is a pendant vertex, $e_u \geq \left\lfloor \frac{m+1}{2} \right\rfloor + 1$, if v is a vertex with degree two, $e_v \geq \left\lfloor \frac{m+1}{2} \right\rfloor$ and if t is a vertex with three degree, $e_t \geq \left\lfloor \frac{m+1}{2} \right\rfloor$. Thus

$$\xi^c(G) = \sum_{u \in V_1(G)} 1.e_u + \sum_{v \in V_2(G)} 2.e_v + \sum_{t \in V_3(G)} 3.e_t$$

$$\geq \sum_{u \in V_1(G)} 1.\left(\left\lfloor \frac{m+1}{2} \right\rfloor + 1 \right) + \sum_{v \in V_2(G)} 2.\left(\left\lfloor \frac{m+1}{2} \right\rfloor \right) + \sum_{t \in V_3(G)} 3.\left(\left\lfloor \frac{m+1}{2} \right\rfloor \right)$$

$$= p\left(\left\lfloor \frac{m+1}{2} \right\rfloor + 1 \right) + 2(2m - 2p)\left(\left\lfloor \frac{m+1}{2} \right\rfloor \right) + 3p\left(\left\lfloor \frac{m+1}{2} \right\rfloor \right)$$

$$= 4m\left\lfloor \frac{m+1}{2} \right\rfloor + p \geq 4m\left\lfloor \frac{m+1}{2} \right\rfloor + 1.$$

If m is odd, then since $m \geq 5$,

$$\xi^c(G) \geq 4m\left(\frac{m+1}{2} \right) + 1 = 2m^2 + 2m + 1 \geq 12m.$$

If m is even, then since $m \geq 5$,

$$\xi^c(G) \geq 4m\left(\frac{m}{2} \right) + 1 = 2m^2 + 1 \geq 12m.$$

The proof is now completed.

The next corollaries are the consequences of Theorem 2.1.

Corollary 2.2. *Let* $G \in U(2m,m) \setminus \{H_1^m\}$, *where* $m \geq 5$. *Then* $\xi^c(G) \geq 12m-1$. *The equality holds if and only if* $G \cong H_2^m$ *or* $G \cong H_3^m$.

Corollary 2.3. *Let* $G \in U(2m,m)$, *where* $m \geq 5$. *Then* $\xi^c(G) \geq 12m-3$. *The equality holds if and only if* $G \cong H_1^m$.

Let A_1^m denote the graph on n vertices obtained from C_3 by attaching $n-2m+1$ pendant edges and $m-2$ paths of length 2 together to one of three vertices of C_3. Let A_2^m denote the graph on n vertices obtained from C_3 by attaching $n-2m+1$ pendant edges and $m-3$ paths of length 2 together to one of three vertices, and two pendant edges to the other two vertices of C_3, respectively. Let A_3^m denote the graph on n vertices obtained from C_3 by attaching $n-2m$ pendant edges and $m-2$ paths of length 2 together to one of three vertices, and a pendant edge to another vertex of C_3, respectively. Let A_4^m denote the graph on n vertices obtained from C_4 by attaching $n-2m+1$ pendant edges and $m-3$ paths of length 2 together with one of the three vertices, and a pendant edge to another vertex of C_4, respectively.

Let A_5^m denote the graph on n vertices obtained from C_4 by attaching $n-2m$ pendant edges and $m-2$ paths of length 2 together to one of three vertices of C_3. A_1^m, A_2^m, A_3^m, A_4^m and A_5^m are shown in Figure 3.

Theorem 2.4. *Let* $G \in U(n,m) \setminus \{A_1^m, A_2^m, A_3^m\}$ $(n \geq 2m,\ m \geq 5)$. *Then* $\xi^c(G) \geq 5n+2m$. *The equality holds if and only if* $G \cong A_4^m$ *or* $G \cong A_5^m$.

Proof. We prove the result by induction on m. If $n = 2m$, then by Theorem 2.1, the result is clear. We assume that $n > 2m$. If $G \cong C_n$, then $n = 2m+1$, since G has an $m-$matching. So, since $m \geq 5$

$$\xi^c(G) = \sum_{u \in V(G)} 2\left\lfloor \frac{2m+1}{2} \right\rfloor = 4m^2 + 2m \geq 5n + 2m.$$

We assume that G ® C_n. By Lemma 1.3, G has an $m-$matching M and pendant vertex v such that M does not saturate v. Let $G' = G - v$. Then $G' \in U(n-1,m)$. Let $e_v = e$ and u be unique neighbor of v pendant vertex. Since $m \geq 4$, then $e \geq 3$. Thus, we have

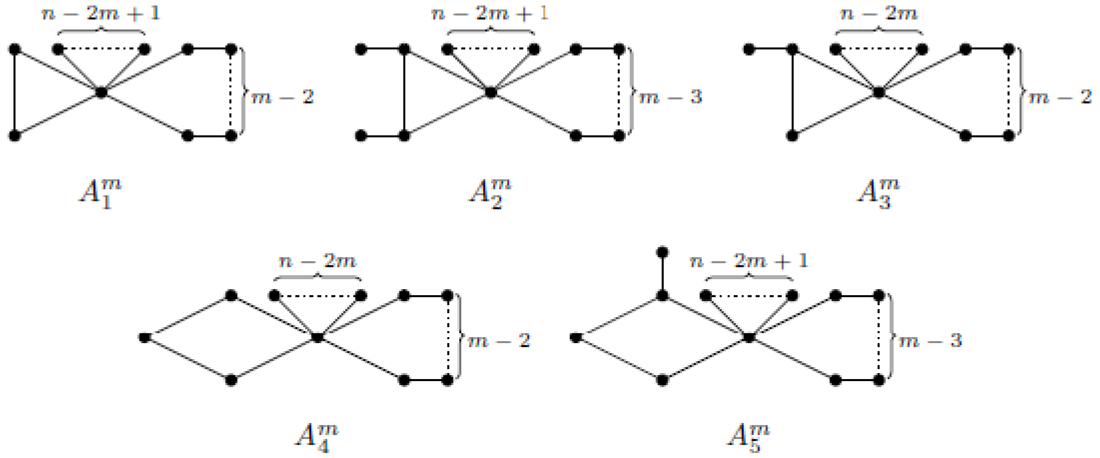


Figure 3

$$\xi^c(G)-\xi^c(G')=1e+d_u(e-1)-(d_u-1)(e-1)+\sum_{t\in V(G)-\{u,v\}} d_t\left[e_t-e_t^{'}\right]$$

$$=2e-1+\sum_{t\in V(G)-\{u,v\}} d_t\left[e_t-e_t^{'}\right]. \qquad (2)$$

Also, we have $0\le e_t-e_t^{'}\le 2.$ Using the equality (2), we get the following inequality

$$\xi^c(G)\ge \xi^c(G^{'})+2e-1.$$

Using the induction hypothesis and the fact $e\ge 3,$ we have

$$\begin{aligned}\xi^c(G)&\ge 5(n-1)+2m+2e-1\\ &=5n+2m+2e-6\\ &\ge 5n+2m.\end{aligned}$$

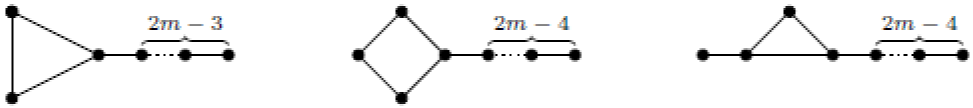
This is the required result.

The next corollaries are the consequences of Theorem 2.4.

Corollary 2.5. *Let* $G\in U(n,m)\setminus\{A_1^m\}\left(n\ge 2m,\ m\ge 5\right).$ *Then* $\xi^c(G)\ge 5n+2m-1.$ *The equality holds if and only if* $G\cong A_2^m$ *or* $G\cong A_3^m.$

Corollary 2.6. *Let* $G\in U(n,m)\setminus\{A_1^m\}\left(n\ge 2m,\ m\ge 5\right).$ *Then* $\xi^c(G)\ge 5n+2m-3.$ *The equality holds if and only if* $G\cong A_1^m.$

Let U_1^m be the graph on $2m$ vertices obtained from C_3 by attaching a path of length $2m-3$ at one vertex. Let U_2^m be the graph on $2m$ vertices obtained from C_4 by attaching a path of length $2m-4$ one vertex. Let U_3^m be the graph on $2m$ vertices obtained from C_3 by attaching a pendant edge at one vertex and a path of length $2m-4$ at one vertex. Denote by U_1^m, U_2^m and U_3^m the graphs shown in Figure 2.



U_1^m U_2^m U_3^m

Figure 4

Theorem 2.7. *Let* $G \in U(2m,m) \setminus \{U_1^m, U_2^m\}$, *where* $m \geq 4$. *Then* $\xi^c(G) \leq 6m^2 - 4m - 7$ *with equality if and only if* $G \cong U_3^m$.

Proof. If $G \cong C_n$, then $\xi^c(G) = 4m^2 \leq 6m^2 - 4m - 7$ for $m \geq 4$. Let G ® C_n. Let G' be a graph obtained from G by using Theorem 1.4. In this case, we obtain $G' \in C_{a,b}(l)$. Then $\xi^c(G) \leq \xi^c(G')$. By applying Lemma 1.5, we get $\xi^c(G) \leq \xi^c(G') \leq \xi^c(U_1^m) = 6m^2 - 4m - 7$. The proof is completed.

The next corollaries are the consequences of Theorem 2.7.

Corollary 2.8. *Let* $G \in U(2m,m) \setminus \{U_1^m\}$, *where* $m \geq 4$. *Then* $\xi^c(G) \leq 6m^2 - 4m - 6$ *with equality if and only if* $G \cong U_2^m$.

In Theorem 1.6, taking $n = 2m$, we have the following corollary.

Corollary 2.9. *Let* $G \in U(2m,m)$, *where* $m \geq 4$. *Then* $\xi^c(G) \leq 6m^2 - 4m - 3$ *with equality if and only if* $G \cong U_1^m$.

Remark 2.10. If $G \in U(2m+1,m)$ By Theorem 1.6, $\xi^c(G) \leq 6m^2 + 2m - 3$ with equality if and only if $G \cong P_n^3$ When $G \in U(n,m)(n \geq 2m+2)$ we do not know upper bounds on $\xi^c(G)$. The case maybe much more complicated.

Remark 2.11. We note that Theorem 2.7 and Corollary 2.9 hold in $U(6,3)$ from the table of connected graphs on six vertices in [4]. But Corollary 2.8 does not hold in case of equality, since $\xi^c(U_2^3) = \xi^c(C_6)$ are in $U(6,3)$.

From the table of unicyclic graphs on eight vertices in [5], we also see that Theorem 2.1 and Corollary 2.3 hold in $U(8,4)$. But Corollary 2.2 does not hold in case of equality, since $\xi^c(H_2^4) = \xi^c(H_3^4) = \xi^c(C_5^*)$ are in $U(8,4)$ where C_5^* is as in Figure 5.

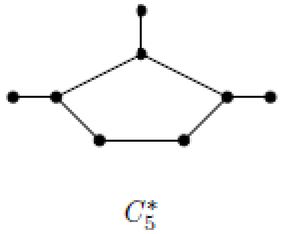


Figure 5

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A Note on Revised Szeged Index of Graph Operations

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ABSTRACT

Let G be a finite and simple graph with edge set $E(G)$. The revised Szeged index is defined as

$$Sz^*(G) = \sum_{e=uv\epsilon E(G)}(n_u(e|G) + \frac{n_G(e)}{2})(n_v(e|G) + \frac{n_G(e)}{2}),$$

where $n_u(e|G)$ denotes the number of vertices in Glying closer to u than to v and $n_G(e)$ is the number of equidistant vertices of e in G. In this paper, we compute the revised Szeged index of the join and corona product of graphs.

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1 INTRODUCTION

Let G be a finite and simple graph with vertex set $V = V(G)$ and edge set $E = E(G)$. The integers $n = n(G) = |V(G)|$ and $m = m(G) = |E(G)|$ are the order and the size of the graph G, respectively. For a vertex $v \in V(G)$, the *open neighborhood* of v, denoted by $N_G(v) = N(v)$ is the set $\{u \in V(G) | uv \in E(G)\}$. The *degree* of $v \in V(G)$, denoted by $d_G(v)$, is defined by $d_G(v) = |N_G(v)|$. Let $u, v \in V(G)$, then the *distance* $d_G(u, v)$ between u and v is defined as the length of any shortest path in G connecting u and v. We consult [14] for notation and terminology which are not defined here.

The first and second Zagreb indices are defined as $M_1(G) = \sum_{u\in V(G)} d_G^2(u)$ and $M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)$, respectively. Furtula and Gutman [5] defined the

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forgotten topological index as $F(G) = \sum_{uv\in E(G)}(d_G^2(u) + d_G^2(v))$. The interested readers are referred to [3,7] for more information on this topic.

A vertex $w \in V(G)$, is said to be equidistant from the edge $e = uv$ of G if $d_G(u,w) = d_G(v,w)$. The number of equidistant vertices of e is denoted by $n_G(e)$. Let uv be an edge of G. Define the sets $N(u,G) = \{x \in V(G) | d_G(u,x) < d_G(v,x)\}$ and $N(v,G) = \{x \in V(G) | d_G(v,x) < d_G(u,x)\}$ consisting, respectively, of vertices of G lying closer to u than to v, and lying closer to v than to u. The number of such vertices is then $n_u(e|G) = |N(u,G)|$ and $n_v(e|G) = |N(v,G)|$. Note that vertices equidistant to u and v are not included into either $N(u,G)$ or $N(v,G)$. It also worth noting that $u \in N(u,G)$ and $v \in N(v,G)$, which implies that $n_u(e|G) \geq 1$ and $n_u(e|G) \geq 1$. The Szeged index $Sz(G)$ was introduced by Gutman [6]. It is defined as $Sz(G) = \sum_{e=uv\in E(G)} n_u(e|G) n_v(e|G)$.

The Szeged index in graphs is well studied in the literature, see for example [9,10]. Randić [13] observed that the Szeged index does not take into account the contributions of the vertices at equal distances from the endpoints of an edge, and so he conceived a modified version of the Szeged index which is named as the revised Szeged index. The revised Szeged index of a connected graph G is defined as $Sz^*(G) = \sum_{e=uv\in E(G)}(n_u(e|G) + \frac{n_G(e)}{2})(n_v(e|G) + \frac{n_G(e)}{2})$. Nagarajan et al. [11] obtained the revised Szeged index of the Cartesian product of two connected graphs. In this paper we compute the revised Szeged index of the join and corona product of graphs. Readers interested in more information on computing topological indices of graph operations can be referred to [1,2,4,8,12].

2. MAIN RESULTS

In this section, we compute the revised Szeged index of the join and corona product of graphs. We let for every edge $e = uv \in E(G)$, $t_{uv}(G) = |N_G(u) \cap N_G(v)|$.

2.1. THE JOIN OF GRAPHS

The join $G = G_1 + G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2. Obviously, $|V(G)| = |V_1| + |V_2|$ and $|E(G)| = |E_1| + |E_2| + |V_1||V_2|$.

Theorem 1. Let G_1 be a graph of order n_1 and of size m_1 and let G_2 be a graph of order n_2 and of size m_2. If $G = G_1 + G_2$, then

$$Sz^*(G) = \frac{2M_2(G_1) + 2M_2(G_2) - n_2M_1(G_1) - n_1M_1(G_2) - F(G_1) - F(G_2)}{4}$$
$$+\frac{4n_1^2n_2^2 + 8m_1m_2 + m_1(n_1^2 + 6n_1n_2 - 3n_2^2) + m_2(n_2^2 + 6n_1n_2 - 3n_1^2)}{4}.$$

Proof. By definition, $Sz^*(G) = \sum_{uv\epsilon E(G)}(n_u(e|G) + \frac{n_G(e)}{2})(n_v(e|G) + \frac{n_G(e)}{2})$. We partition the edges of G in to three subset E_1, E_2 and E_3, as $E_1 = \{e = uv \mid u, v \in V(G_1)\}$, $E_2 = \{e = uv \mid u, v \in V(G_2)\}$ and $E_3 = \{e = uv \mid u \in V(G_1), v \in V(G_2)\}$.

Let $e = uv \in E_1$. If $w \in V(G_2)$ or $w \in N_{G_1}(u) \cap N_{G_1}(v)$, then $d_G(u,w) = d_G(v,w) = 1$ and if $w \notin N_{G_1}(u) \cup N_{G_1}(v)$, then $d_G(u,w) = d_G(v,w) = 2$. Hence $n_u(e|G) = d_{G_1}(u) - t_{uv}(G_1) + 1, n_v(e|G) = d_{G_1}(v) - t_{uv}(G_1) + 1$ and $n_G(e) = n_1 + n_2 + 2t_{uv}(G_1) - \left(d_{G_1}(u) + d_{G_1}(v)\right) - 2$. Then for every edge $e = uv \in E_1$,

$$\begin{aligned}\left(n_u(e|G) + \frac{n_G(e)}{2}\right)\left(n_v(e|G) + \frac{n_G(e)}{2}\right) &= \left(\frac{n_1+n_2+d_{G_1}(u)-d_{G_1}(v)}{2}\right)\left(\frac{n_1+n_2+d_{G_1}(v)-d_{G_1}(u)}{2}\right)\\ &= \frac{(n_1+n_2)^2}{4} + \frac{d_{G_1}(u)d_{G_1}(v)}{2} - \frac{d_{G_1}^2(u)+d_{G_1}^2(v)}{4}.\end{aligned}$$

Therefore

$$\begin{aligned}\sum_{uv\epsilon E_1}\left(n_u(e|G) + \frac{n_G(e)}{2}\right)\left(n_v(e|G) + \frac{n_G(e)}{2}\right) &= \sum_{uv\epsilon E_1}\frac{(n_1+n_2)^2}{4} + \sum_{uv\epsilon E_1}\frac{d_{G_1}(u)d_{G_1}(v)}{2}\\ &\quad - \sum_{uv\epsilon E_1}\frac{d_{G_1}^2(u)+d_{G_1}^2(v)}{4}\\ &= \frac{(n_1+n_2)^2}{4}m_1 + \frac{M_2(G_1)}{2} - \frac{F(G_1)}{4}. \qquad (1)\end{aligned}$$

Similarly,

$$\sum_{uv\epsilon E_2}\left(n_u(e|G) + \frac{n_G(e)}{2}\right)\left(n_v(e|G) + \frac{n_G(e)}{2}\right) = \frac{(n_1+n_2)^2}{4}m_2 + \frac{M_2(G_2)}{2} - \frac{F(G_2)}{4}\,. \qquad (2)$$

Let $e = uv \in E_3$ such that $u \in V(G_1)$ and $v \in V(G_2)$. If $w \in N_{G_1}(u) \cup N_{G_2}(v)$, then $d_G(u,w) = d_G(v,w) = 1$. Hence $n_u(e|G) = n_2 - d_{G_2}(v) + 1, n_v(e|G) = n_1 - d_{G_1}(u) + 1$ and $n_G(e) = d_{G_1}(u) + d_{G_2}(v) - 2$. Then for every edge $e = uv \in E_3$,

$$\begin{aligned}\left(n_u(e|G) + \frac{n_G(e)}{2}\right)\left(n_v(e|G) + \frac{n_G(e)}{2}\right) &= \left(\frac{2n_2+d_{G_1}(u)-d_{G_2}(v)}{2}\right)\left(\frac{2n_1+d_{G_2}(v)-d_{G_1}(u)}{2}\right)\\ &= n_1n_2 + \frac{n_1-n_2}{2}d_{G_1}(u) + \frac{n_2-n_1}{2}d_{G_2}(v)\\ &\quad - \frac{d_{G_1}^2(u)}{4} - \frac{d_{G_2}^2(v)}{4} + \frac{d_{G_1}(u)d_{G_2}(v)}{2}.\end{aligned}$$

Set $Y = \sum_{uv\epsilon E_3}\left(n_u(e|G) + \frac{n_G(e)}{2}\right)\left(n_v(e|G) + \frac{n_G(e)}{2}\right)$. Then,

$$\begin{aligned}Y &= \sum_{uv\epsilon E_3} n_1n_2 + \sum_{uv\epsilon E_3}\frac{n_1-n_2}{2}d_{G_1}(u) + \sum_{uv\epsilon E_3}\frac{n_2-n_1}{2}d_{G_2}(v) - \sum_{uv\in E_3}\frac{d_{G_1}^2(u)}{4}\\ &\quad - \sum_{uv\epsilon E_3}\frac{d_{G_2}^2(v)}{4} + \sum_{uv\epsilon E_3}\frac{d_{G_1}(u)d_{G_2}(v)}{2}\end{aligned}$$

$$= n_1^2 n_2^2 + m_1 n_2(n_1 - n_2) + m_2 n_1(n_2 - n_1) + 2m_1 m_2 - \frac{n_2 M_1(G_1)}{4} - \frac{n_1 M_1(G_2)}{4}. \qquad (3)$$

By Equations (1), (2) and (3), we have:

$$\begin{aligned} Sz^*(G) = {} & \frac{(n_1+n_2)^2}{4} m_1 + \frac{M_2(G_1)}{2} - \frac{F(G_1)}{4} + \frac{(n_1+n_2)^2}{4} m_2 + \frac{M_2(G_2)}{2} - \frac{F(G_2)}{4} + n_1^2 n_2^2 + 2\mathrm{m}_1\mathrm{m}_2 \\ & - \frac{n_1 M_1(G_2)}{4} + m_1 n_2(n_1 - n_2) + m_2 n_1(n_2 - n_1) - \frac{n_2 M_1(G_1)}{4} \\ = {} & \frac{2M_2(G_1) + 2M_2(G_2) - n_2 M_1(G_1) - n_1 M_1(G_2) - F(G_1) - F(G_2)}{4} \\ & + \frac{4n_1^2 n_2^2 + 8m_1 m_2 + m_1(n_1^2 + 6n_1 n_2 - 3n_2^2) + m_2(n_2^2 + 6n_1 n_2 - 3n_1^2)}{4}. \end{aligned}$$

Let P_n, $n \geq 2$ and C_n, $n \geq 3$ denote the path and the cycle on n vertices, respectively.

Corollary 2. The following equalities are hold:

1. $Sz^*(P_n + P_m) = \frac{4n^2m^2 + n^3 + m^3 + 3nm^2 + 3mn^2 + 2n^2 + 2m^2 - 2n - 2m - 12nm + 4}{4}$.
2. $Sz^*(P_n + C_m) = \frac{4n^2m^2 + n^3 + m^3 + 3nm^2 + 3mn^2 - n^2 + 3m^2 - 2m - 6nm - 2}{4}$.
3. $Sz^*(C_n + C_m) = \frac{4n^2m^2 + n^3 + m^3 + 3nm^2 + 3mn^2}{4}$.

2.2. THE CORONA PRODUCT OF GRAPHS

The corona product $G = G_1 o G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is as the graph obtained by taking one copy of G_1 and $|V_1|$ copies of G_2 and joining the i-th vertex of G_1 to every vertex in i-th copy of G_2. Obviously, $|V(G)| = |V_1| + |V_1||V_2|$ and $|E(G)| = |E_1| + |V_1||E_2| + |V_1||V_2|$.

Theorem 3. Let G_1 be a graph of order n_1 and of size m_1 and let G_2 be a graph of order n_2 and of size m_2. If $G = G_1 o G_2$, then

$$\begin{aligned} Sz^*(G) = {} & \frac{(n_1 n_2 + n_1)^2}{4}(m_1 + m_2) + n_1 n_2(n_1 n_2 + n_1 - 1) \\ & + n_1 m_2(n_1 n_2 + n_1 - 2) - \frac{(n_2+1)^2}{4} \sum_{uv \in E_1} (n_u^2(e|G_1) + n_v^2(e|G_1)) \\ & + \frac{2(n_2+1)^2 \mathrm{Sz}(G_1) + 2M_2(G_2) - n_1 M_1(G_2) - F(G_2)}{4}. \end{aligned}$$

Proof. By definition, $Sz^*(G) = \sum_{uv \epsilon E(G)} (n_u(e|G) + \frac{n_G(e)}{2})(n_v(e|G) + \frac{n_G(e)}{2})$. We partition the edges of G in to three subsets E_1, E_2 and E_3, as $E_1 = \{e = uv \mid u, v \in V(G_1)\}$, $E_2 = \{e = uv \mid u, v \in V(G_2)\}$ and $E_3 = \{e = uv \mid u \in V(G_1), v \in V(G_2)\}$. Let $e = uv \in E_1$. Then for each vertex w closer to u than v, the vertices of the copy of G_2 attached to w are also closer to u than v. Since each copy of G_2 has exactly n_2 vertices, then $n_u(e|G) = (n_2+1)n_u(e|G_1)$. Similarly $n_v(e|G) = (n_2+1)n_v(e|G_1)$. Then $n_G(e) = n_1n_2 + n_1 - (n_2+1)n_u(e|G_1) - (n_2+1)n_v(e|G_1)$. Hence for every edge $e = uv \in E_1$,

$$\left(n_u(e|G) + \frac{n_G(e)}{2}\right)\left(n_v(e|G) + \frac{n_G(e)}{2}\right) = \frac{(n_1n_2+n_1)^2}{4} + \frac{(n_2+1)^2 n_u(e|G_1)n_v(e|G_1)}{2} - \frac{(n_2+1)^2(n_u^2(e|G_1)+n_v^2(e|G_1))}{4}.$$

Define $Z = \sum_{uv\epsilon E_1}\left(n_u(e|G) + \frac{n_G(e)}{2}\right)\left(n_v(e|G) + \frac{n_G(e)}{2}\right)$. Then,

$$\begin{aligned} Z &= \sum_{uv\epsilon E_1}\frac{(n_1n_2+n_1)^2}{4} + \sum_{uv\epsilon E_1}\frac{(n_2+1)^2 n_u(e|G_1)n_v(e|G_1)}{2} - \sum_{uv\epsilon E_1}\frac{(n_2+1)^2(n_u^2(e|G_1)+n_v^2(e|G_1))}{4} \\ &= \frac{(n_1n_2+n_1)^2}{4}m_1 + \frac{(n_2+1)^2 Sz(G_1)}{2} - \frac{(n_2+1)^2}{4}\sum_{e=uv\epsilon E_1}(n_u^2(e|G_1) + n_v^2(e|G_1)). \end{aligned} \qquad (4)$$

Let $e = uv \in E_2$. If $w \in V(G_2)$ and $w \in N_{G_2}(u) \cap N_{G_2}(v)$, then $d_G(u,w) = d_G(v,w) = 1$ and if $w \notin N_{G_2}(u) \cup N_{G_2}(v)$, then $d_G(u,w) = d_G(v,w) = 2$. Hence $n_u(e|G) = d_{G_2}(u) - t_{uv}(G_2) + 1, n_v(e|G) = d_{G_2}(v) - t_{uv}(G_2) + 1$ and $n_G(e) = n_1n_2 + n_1 + 2t_{uv}(G_2) - \left(d_{G_2}(u) + d_{G_2}(v)\right) - 2$. Hence for every edge $e = uv \in E_2$,

$$\begin{aligned} \left(n_u(e|G) + \frac{n_G(e)}{2}\right)\left(n_v(e|G) + \frac{n_G(e)}{2}\right) &= \left(\frac{n_1n_2+n_1+d_{G_2}(u)-d_{G_2}(v)}{2}\right)\left(\frac{n_1n_2+n_1+d_{G_2}(v)-d_{G_2}(u)}{2}\right) \\ &= \frac{(n_1n_2+n_1)^2}{4} + \frac{d_{G_2}(u)d_{G_2}(v)}{2} - \frac{d_{G_2}^2(u)+d_{G_2}^2(v)}{4}. \end{aligned}$$

Therefore

$$\begin{aligned} \sum_{uv\epsilon E_2}\left(n_u(e|G) + \frac{n_G(e)}{2}\right)\left(n_v(e|G) + \frac{n_G(e)}{2}\right) &= \sum_{uv\epsilon E_2}\frac{(n_1n_2+n_1)^2}{4} + \sum_{uv\epsilon E_2}\frac{d_{G_2}(u)d_{G_2}(v)}{2} \\ &\quad - \sum_{uv\epsilon E_2}\frac{d_{G_2}^2(u)+d_{G_2}^2(v)}{4} \\ &= \frac{(n_1n_2+n_1)^2}{4}m_2 + \frac{M_2(G_2)}{2} - \frac{F(G_2)}{4}. \end{aligned} \qquad (5)$$

Let $e = uv \in E_3$ such that $u \in V(G_1)$ and $v \in V(G_2)$. Hence $n_u(e|G) = n_1n_2 + n_1 - d_{G_2}(v) - 1$. Since $v \in N(v,G)$, we have $n_v(e|G) = 1$ and so $n_G(e) = d_{G_2}(v)$. Hence

$$\begin{aligned} \left(n_u(e|G) + \frac{n_G(e)}{2}\right)\left(n_v(e|G) + \frac{n_G(e)}{2}\right) &= \left(\frac{2(n_1n_2+n_1-1)-d_{G_2}(v)}{2}\right)\left(\frac{2+d_{G_2}(v)}{2}\right) \\ &= (n_1n_2 + n_1 - 1) + \frac{n_1n_2+n_1-2}{2}d_{G_2}(v) - \frac{d_{G_2}^2(v)}{4}. \end{aligned}$$

Therefore,

$$\begin{aligned} \sum_{uv\epsilon E_3}\left(n_u(e|G) + \frac{n_G(e)}{2}\right)\left(n_v(e|G) + \frac{n_G(e)}{2}\right) &= \sum_{uv\epsilon E_3}(n_1n_2 + n_1 - 1) - \sum_{uv\epsilon E_3}\frac{d_{G_2}^2(v)}{4} \\ &\quad + \sum_{e=uv\epsilon E_3}\frac{n_1n_2+n_1-2}{2}d_{G_2}(v) \end{aligned}$$

$$= n_1n_2(n_1n_2 + n_1 - 1) - \frac{n_1M_1(G_2)}{4}$$
$$+n_1m_2(n_1n_2 + n_1 - 2). \qquad (6)$$

By Equations (4), (5) and (6), we have:

$$\begin{aligned} Sz^*(G) &= \frac{(n_1n_2+n_1)^2}{4}m_1 + \frac{(n_2+1)^2Sz(G_1)}{2} - \frac{(n_2+1)^2}{4}\sum_{uv\epsilon E_1}(n_u^2(e|G_1) + n_v^2(e|G_1)) \\ &+ \frac{(n_1n_2+n_1)^2}{4}m_2 + \frac{M_2(G_2)}{2} - \frac{F(G_2)}{4} + n_1n_2(n_1n_2 + n_1 - 1) \\ &+n_1m_2(n_1n_2 + n_1 - 2) - \frac{n_1M_1(G_2)}{4} \\ &= \frac{(n_1n_2+n_1)^2}{4}(m_1 + m_2) + n_1n_2(n_1n_2 + n_1 - 1) \\ &+n_1m_2(n_1n_2 + n_1 - 2) - \frac{(n_2+1)^2}{4}\sum_{uv\in E_1}(n_u^2(e|G_1) + n_v^2(e|G_1)) \\ &+ \frac{2(n_2+1)^2\mathrm{Sz}(G_1)+2M_2(G_2)-n_1M_1(G_2)- F(G_2)}{4}. \end{aligned}$$

Corollary 4. The following equalities are hold:

1. $Sz^*(P_noP_m)= \frac{2n^3m^2+3n^2m^3+24n^2m^2+4n^3m-2nm^2+2n^3+15mn^2-15n^2+40n-52nm-6}{4}.$
2. $Sz^*(P_noC_m)= \frac{2n^3m^2+2n^2m^3+28n^2m^2+4n^3m-2nm^2+2n^3+26mn^2-2n-52nm}{4}.$
3. $Sz^*(C_noP_m)= \frac{n^3m^2+n^2m^3+9n^2m^2+2n^3m+n^3+3mn^2-5n^2-16nm-2n-2}{4}.$
4. $Sz^*(C_noC_m)= \frac{n^3m^2+n^2m^3+10n^2m^2+2n^3m+n^3+9mn^2-16nm}{4}.$

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Weak Chemical Hyperstructures Associated to Electrochemical Cells

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ABSTRACT

Algebraic hyperstructures have many applications in various sciences. The main purpose of this paper is to provide a new application of weak hyperstructures in Chemistry. More precisely, we present three different examples of hyperstructures associated to electrochemical cells. In which we prove that our hyperstructures are H_v -semigroups and we present some interesting results.

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1 INTRODUCTION

Hyperstructures represent a natural extension of algebraic structures and they were introduced in 1934 by F. Marty [14]. He generalized the notion of groups by defining hypergroups. Where in a group, the operation's result of two elements is again an element while in a hypergroup, the hyperoperation's result of two elements is a non-void set. Since then, hundred of books and papers discussed and studied hyperstructures from the theoretical point of view and for their applications to many subjects of pure and applied mathematics. In [5], Corsini presented some of hyperstructures' applications to several subjects such as, geometry, fuzzy sets, automata, hypergraphs, and so on.

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The largest class of hyperstructures is the one that satisfies weak axioms, i.e., the non-empty intersection replaces the equality. These are called Hv-structures and they were introduced in 1990. The latter hyperstructures have many applications to different disciplines like Biology, Chemistry, Physics, and so on. In [1, 2], the authors analyzed the second generation phenotypes and genotypes of n-hybrid cross with a mathematical structure. They used the concepts of cyclic hypergroup and H_v-semigroup in the F_2-phenotypes and F_2-genotypes respectively with mating as a hyperoperation. Another motivation for the study of hyperstructures comes from chemical reactions. In [3, 6, 7, 8], redox, chain and dismutation reactions were provided as different examples of weak hyperstructures.

In our paper, we consider a new chemical hyperstructure using Galvanic and Electrolytic cells. And it is organized as follows: after an introduction, Section 2 presents some definitions that are used throughout the paper. Section 3 defines binary hyperstructures related to Galvanic cells, Electrolytic cells and proves that they are isomorphic. Moreover, it defines a binary hyperstructure related to both Galvanic and Electrolytic cells at the same time and investigate its properties.

2. WEAK HYPERSTRUCTURES

In this section, we present some definitions related to hyperstructures (see [4, 9, 10, 11, 12, 13]) that are used throughout the paper.

Let H be a non-empty set. Then, a mapping $\circ : H \times H \to P^*(H)$ is called a binary hyperoperation on H, where $P^*(H)$ is the family of all non-empty subsets of H. The couple $(H,\circ)$ is called a hypergroupoid. In the above definition, if A and B are two non-empty subsets of H and $x \in H$, then we define: $A \circ B = \bigcup_{a\in A, b\in B} a \circ b$, $x \circ A = \{x\} \circ A$ and $A \circ x = A \circ \{x\}$.

H_v-structures were introduced by T. Vougiouklis as a generalization of the well-known algebraic hyperstructures. Some axioms of classical algebraic hyperstructures are replaced by their corresponding weak axioms in H_v-structures. Most of H_v-structures are used in representation theory.

A hypergroupoid $(H,\circ)$ is called an H_v-semigroup if for all $x, y, z \in H$,

$$\big(x \circ (y \circ z)\big) \cap \big((x \circ y) \circ z\big) \neq \emptyset.$$

A subset K of an H_v-semigroup is an H_v-subsemigroup if K is an H_v-semigroup. An element $x \in H$ is called idempotent if $x^2 = x \circ x = x$ and an element $e \in H$ is called an identity of (H,∘) if $x \in x \circ e \cap e \circ x$, for all $x \in H$. The latter is called strong identity if $e \circ x = x \circ e \subseteq \{e, x\}$ for all $x \in H$. A hypergroupoid $(H,\circ)$ is called a semihypergroup if for every $x, y, z \in H$, we have $x \circ (y \circ z) = (x \circ y) \circ$

z and is called a quasihypergroup if for every $x \in H$, $x \circ H = H = H \circ x$. The latter condition is called the reproduction axiom. The couple $(H,\circ)$ is called a hypergroup if it is a semihypergroup and a quasi-hypergroup. Two hypergroupoids $(H,\circ)$ and $(K,*)$ are said to be isomorphic hypergroupoids, written as $H \cong K$, if there exists a bijective function $f\colon H \to K$ such that $f(x \circ y) = f(x) * f(y)$ for all $x, y \in H$.

3. MAIN RESULTS

This section is divided into three subsection as Galvanic Cells , Electrolytic Cells and Galvanic/Electrolytic Cells. Each section will be separately discussed in what follows:

3.1. GALVANIC CELLS

Chemical reactions involving the transfer of electrons from one reactant to another are called oxidation-reduction reactions or redox reactions. In a redox reaction, two half-reactions occur; one reactant (with less electronegativity) gives up electrons (undergoes oxidation) and another reactant (with higher electronegativity) gains electrons (undergoes reduction). For example, a piece of zinc going into a solution as zinc ions, with each Zn atom giving up 2 electrons, is an example of an oxidation half-reaction.

$$Zn \to Zn^{2+} + 2e^{-}.$$

In contrast, the reverse reaction, in which Zn^{2+} ions gain 2 electrons to become Zn atoms, is an example of a reduction half-reaction.

$$Zn^{2+} + 2e^{-} \to Zn.$$

A redox reaction result when an oxidation and reduction half-reaction are combined to complete a transfer of electrons as in the following example:

$$Zn + Cu^{2+} \to Zn^{2+} + Cu.$$

The electrons are not shown in the above redox reaction because they are neither reactants nor products but have simply been transferred from one species to another (from Zn to Cu^{2+} in this case). In this redox reaction, the Zn is referred to as the reducing agent because it causes the Cu^{2+} to be reduced to Cu. The Cu^{2+} is called the oxidizing agent because it causes the Zn to be oxidized to Zn^{2+}.

A Galvanic cell or voltaic cell is a device in which a redox reaction spontaneously occurs and produces an electric current. In order for the transfer of electrons in a redox reaction to produce an electric current and be useful, the electrons are made to pass through an external electrically conducting wire instead of being directly transferred between the oxidizing and reducing agents. The design of a Galvanic cell allows this to occur. In a Galvanic cell, two solutions, one containing the ions of the oxidation half-reaction and the other containing the ions of the reduction half-reaction, are placed in separated compartments called half-cells. For each half-cell, the metal, which is called an electrode, is placed in the solution and connected to an external wire. The electrode at which oxidation occurs is called the anode (Zn in the above example) and the electrode at which reduction occurs is called the cathode (Cu in the above example). The two half-cells are connected by a salt-bridge that allows a “current” of ions from one half-cell to the other to complete the circuit of electron current in the external wires. When the two electrodes are connected to an electric load (such as a light bulb or voltmeter) the circuit is completed, the oxidation-reduction reaction occurs, and electrons move from the anode (-) to the cathode (+), producing an electric current.

Galvanic cell consists of two half-cells, such that the electrode of one half-cell is composed of metal A (with larger electronegativity) and the electrode of the other half-cell is composed of metal B (with smaller electronegativity). The redox reactions for the two separate half-cells are given as follows:

$$A^{n+} + ne^- \to A,$$
$$B \to B^{m+} + me^-.$$

The two metals A and B can react with each other according to the following balanced equation:

$$nB + mA^{n+} \to mA + nB^{m+}.$$

Having the element Cu with greater electronegativity than that of Zn, we get that $Zn + Cu^{2+} \to Zn^{2+} + Cu$ is an example of a redox reaction occurring in a Galvanic cell. For more details about Galvanic cells, see [16].

Next, we present a commutative hyperstructure related to Galvanic cell and investigate its properties. We consider the set $H = \{A, B, A^{n+}, B^{m+}\}$ and we define a hyperoperation $\oplus_1$ on H as follows: $x \oplus_1 y$ is the result of a possible reaction between x and y in a Galvanic cell. If x and y do not react in a Galvanic cell then we set $x \oplus_1 y = \{x, y\}$. All possible spontaneous redox reactions of $\{A, B, A^{n+}, B^{m+}\}$ in a Galvanic cell are summarized in the following commutative table:

$\oplus_1$	A	B	A^{n+}	B^{m+}
A	A	$\{A,B\}$	$\{A, A^{n+}\}$	$\{A, B^{m+}\}$
B	$\{A, B\}$	B	$\{A, B^{m+}\}$	$\{B, B^{m+}\}$
A^{n+}	$\{ A, A^{n+}\}$	$\{A, B^{m+}\}$	A^{n+}	$\{ A^{n+}, B^{m+}\}$
B^{m+}	$\{A, B^{m+}\}$	$\{B, B^{m+}\}$	$\{ A^{n+}, B^{m+}\}$	B^{m+}

In above table, if we change the names from A, B, A^{n+}, B^{m+} to a, b, c, d respectively, then the following theorem holds.

Theorem 1. Let $H=\{a, b, c, d\}$, $\oplus_1$ be the hyperoperation on H and consider the following table corresponding to $(H,\oplus_1)$:

$\oplus_1$	a	b	c	d
a	a	$\{a, b\}$	$\{a, c\}$	$\{a, \mathrm{d}\}$
b	$\{a, b\}$	b	$\{a, d\}$	$\{b, d\}$
c	$\{a, c\}$	$\{a, d\}$	c	$\{c, \mathrm{d}\}$
d	$\{a, d\}$	$\{b, d\}$	$\{c, d\}$	d

Then $(H,\oplus_1)$ is a commutative H_v-semigroup.

Proof. It is clear from the above table that $(H,\oplus_1)$ is a commutative hypergroupoid. We need to show that $(H,\oplus_1)$ is a weak associative hypergroupoid, i.e, $x \oplus_1 (y \oplus_1 z) \cap (x \oplus_1 y) \oplus_1 z \neq \emptyset$ for all $(x, y, z) \in H^3$. We have three cases for x; $x = a \text{ or } d$, $x = b$ and $x = c$:

- Case $x = a \text{ or } d$. We have that $x \in x \oplus_1 (y \oplus_1 z) \cap (x \oplus_1 y) \oplus_1 z \neq \emptyset$.
- Case $x = b$. We have that $b \oplus_1 (c \oplus_1 c) = b \oplus_1 c = \{a, d\}$ and that $(b \oplus_1 c) \oplus_1 c = \{a, d\} \oplus_1 c = \{a, c, d\}$. Thus,
  $$b \oplus_1 (c \oplus_1 c)(b \oplus_1 c) \oplus_1 c \neq \emptyset.$$
  Moreover, one can easily check that $b \oplus_1 (c \oplus_1 z) \cap (b \oplus_1 c) \oplus_1 z \neq \emptyset$, and that $b \oplus_1 (y \oplus_1 c) \cap (b \oplus_1 y) \oplus_1 c \neq \emptyset$. If $y \neq c$ and $z = c$ then $b \in b \oplus_1 (y \oplus_1 z) \cap (b \oplus_1 y) \oplus_1 z$.
- Case $x = c$. This case is similar to that of Case $x = b$.

Remark 1. Since $a \oplus_1 (b \oplus_1 c) = \{a, d\} \neq (a \oplus_1 b) \oplus_1 c = \{a, c, d\}$, it follows that $(H,\oplus_1)$ is not a semihypergroup.

Remark 2. $(H,\oplus_1)$ admits two identities; a and d. Moreover, a and d are strong identities.

3.2. ELECTROLYTIC CELLS

Voltaic cells are driven by a spontaneous chemical reaction that produces an electric current through an outside circuit. These cells are important because they are the basis for the batteries that fuel modern society. But they aren't the only kind of electrochemical cells. The reverse reaction in each case is non-spontaneous and requires electrical energy to occur. It is possible to construct a cell that does work on a chemical system by driving an electric current through the system. These cells are called electrolytic cells (or reverse Galvanic cells), and operate through electrolysis.

Electrolysis is used to drive an oxidation-reduction reaction in a direction in which it does not occur spontaneously by driving an electric current through the system while doing work on the chemical system itself, and therefore is non-spontaneous. Electrolytic cells, like Galvanic cells, are composed of two half-cells; one is a reduction half-cell, the other is an oxidation half-cell. The direction of electron flow in electrolytic cells, however, may be reversed from the direction of spontaneous electron flow in Galvanic cells, but the definition of both cathode and anode remain the same, where reduction takes place at the cathode and oxidation occurs at the anode. Because the directions of both half-reactions have been reversed, the sign, but not the magnitude, of the cell potential has been reversed.

Electrolytic cells consist of two half-cells, such that the electrode of one half-cell is composed of metal A (with larger electronegativity) and the electrode of the other half-cell is composed of metal B (with smaller electronegativity). The redox reactions for the two separate half-cells are given as follows:

$$A \to A^{n+} + ne^-,$$

$$B^{m+} + me^- \to B.$$

The two metals A and B can react with each other according to the following balanced equation:

$$mA + nB^{m+} \to nB + mA^{n+}.$$

An example of a reaction in an Electrolytic cell is:

$$Cu + Zn^{2+} \to Zn + Cu^{2+}$$

which is the reverse of the reaction described before. For more details about Electrolytic cells, see [16].

Next we present a hyperstructure related to Electrolytic cells and investigate its properties. We consider the set $H= \{A, B, A^{n+}, B^{m+}\}$ and we define a hyperoperation $\oplus_2$ on H as follows: $x \oplus_2 y$ is the result of a possible reaction between x and y in an Electrolytic cell. If x and y do not react in an electrolytic cell then we set $x \oplus_2 y = \{x, y\}$.

All possible spontaneous redox reactions of $\{A, B, A^{n+}, B^{m+}\}$ in an electrolytic cell are summarized in the following commutative table:

$\oplus_2$	A	B	A^{n+}	B^{m+}
A	A	$\{A, B\}$	$\{A, A^{n+}\}$	$\{A^{n+}, B\}$
B	$\{A, B\}$	B	$\{A^{n+}, B\}$	$\{B, B^{m+}\}$
A^{n+}	$\{A, A^{n+}\}$	$\{A^{n+}, B\}$	A^{n+}	$\{A^{n+}, B^{m+}\}$
B^{m+}	$\{A^{n+}, B\}$	$\{B, B^{m+}\}$	$\{A^{n+}, B^{m+}\}$	B^{m+}

In the above table, if we change the names from A, B, A^{n+}, B^{m+} to a, b, c, d respectively, then the following theorem holds.

Theorem 2. Let $H=\{a, b, c, d\}$, $\oplus_2$ be the hyperoperation on H and consider the following table corresponding to $(H,\oplus_2)$:

$\oplus_2$	a	b	c	d
a	a	$\{a, b\}$	$\{a, c\}$	$\{b, c\}$
b	$\{a, b\}$	b	$\{b, c\}$	$\{b, \mathrm{d}\}$
c	$\{a, c\}$	$\{b, c\}$	c	$\{c, d\}$
d	$\{b, c\}$	$\{b, d\}$	$\{c, d\}$	d

Then $(H,\oplus_2)$ is a commutative H_v-semigroup.

Proof. Let $f: (H,\oplus_1) \to (H,\oplus_2)$ defined as follows:

$$f(a) = b, f(b) = a, f(c) = d \text{ and } f(d) = c.$$

It is easy to see that f is an isomorphism and thus, $(H,\oplus_1) \cong (H,\oplus_2)$. The latter and Theorem 1 imply that $(H,\oplus_2)$ is a commutative H_v-semigroup.

Remark 3. $(H,\oplus_2)$ admits two identities; b and c. Moreover, b and c are strong identities.

3.3. GALVANIC/ELECTROLYTIC CELLS

We present a commutative hyperstructure related to Galvanic/Electrolytic cells and investigate its properties. We consider the set $H=\{A, B, A^{n+}, B^{m+}\}$ and we define a hyperoperation $\oplus$ on H as follows: $x \oplus y$ is the result of a possible reaction between x and y in either a Galvanic cell or in an Electrolytic cell. If x and y neither react in a Galvanic cell nor in an Electrolytic cell then we set $x \oplus y = \{x, y\}$.

All possible spontaneous redox reactions of $\{A, B, A^{n+}, B^{m+}\}$ in a Galvanic/Electrolytic cell are summarized in the following commutative table:

$\oplus$	A	B	A^{n+}	B^{m+}
A	A	$\{A, B\}$	$\{A, A^{n+}\}$	$\{A^{n+}, B\}$
B	$\{A, B\}$	B	$\{A, B^{m+}\}$	$\{B, B^{m+}\}$
A^{n+}	$\{A, A^{n+}\}$	$\{A, B^{m+}\}$	A^{n+}	$\{A^{n+}, B^{m+}\}$
B^{m+}	$\{A^{n+}, B\}$	$\{B, B^{m+}\}$	$\{A^{n+}, B^{m+}\}$	B^{m+}

Remark 4. We can define $(H,\oplus)$ as follows:

$$x \oplus y = \begin{cases} x \oplus_1 y & \text{if } x \oplus_2 y = \{x,y\}; \\ x \oplus_2 y & \text{if } x \oplus_1 y = \{x,y\}; \\ \{x,y\} & \text{if } x \oplus_1 y = x \oplus_2 y. \end{cases}$$

In the above table, if we change the names from *A, B,* A^{n+}, B^{m+} to *a, b, c, d* respectively, then the following theorem holds.

Theorem 3. Let $H=\{a, b, c, d\}$, $\oplus$ be the hyperoperation on H and consider the following table corresponding to $(H,\oplus)$:

$\oplus$	a	b	c	d
a	a	$\{a, b\}$	$\{a, c\}$	$\{b, c\}$
b	$\{a, b\}$	b	$\{a, d\}$	$\{b, d\}$
c	$\{a, c\}$	$\{a, d\}$	c	$\{c, d\}$
d	$\{b, c\}$	$\{b, d\}$	$\{c, d\}$	d

Then $(H,\oplus)$ is a commutative H_v-semigroup.

Proof. It is clear from the above table that $(H,\oplus)$ is a commutative hypergroupoid. We need to show that $(H,\oplus)$is a weak associative hypergroupoid. Let $(x,y,z) \in H^3$. We have four cases for *x; x=a, x=b, x=c* and *x=d*:

- Case $x = a$. We have that $a \oplus (d \oplus d) = a \oplus d = \{b,c\}$ and that $(a \oplus d) \oplus d = \{b,c\} \oplus d = \{b,c,d\}$. Thus, $a \oplus (d \oplus d) \cap (a \oplus d) \oplus d \neq \emptyset$. Moreover, one can easily check that $a \oplus (d \oplus z) \cap (a \oplus d) \oplus z$ and that $a \oplus (y \oplus d) \cap (a \oplus y) \oplus d \neq \emptyset$. If $y \neq d$ and $z \neq d$ then $a \in a \oplus (y \oplus z) \cap (a \oplus y) \oplus z$.
- Case $x = b$. We have that $b \oplus (c \oplus c) = b \oplus c = \{a,d\}$ and that $(b \oplus c) \oplus c = \{a,d\} \oplus c = \{a,c,d\}$. Thus, $b \oplus (c \oplus c) \cap (b \oplus c) \oplus c \neq \emptyset$. Moreover, one can easily check that $b \in b \oplus (c \oplus z) \cap (b \oplus c) \oplus z \neq \emptyset$ and that $b \oplus (y \oplus c) \cap (a \oplus y) \oplus c \neq \emptyset$. If $y \neq c$ and $z \neq c$ then $b \in b \oplus (y \oplus z) \cap (b \oplus y) \oplus z$.
- Case $x = c$. We have that $c \oplus (b \oplus b) = c \oplus b = \{a,d\}$ and that $(c \oplus b) \oplus b = \{a,d\} \oplus b = \{a,b,d\}$. Thus, $c \oplus (b \oplus b) \cap (c \oplus b) \oplus b \neq \emptyset$. Moreover, one can easily check that $c \oplus (b \oplus z) \cap (c \oplus b) \oplus z \neq \emptyset$ and that $c \oplus (y \oplus b) \cap (c \oplus y) \oplus b \neq \emptyset$. If $y \neq b$ and $z \neq b$ then $c \in c \oplus (y \oplus z) \cap (c \oplus y) \oplus z$.
- Case $x = d$. We have that $d \oplus (a \oplus a) = d \oplus a = \{b,c\}$ and that $(d \oplus a) \oplus a = \{b,c\} \oplus a = \{a,b,c\}$. Thus, $d \oplus (a \oplus a) \cap (d \oplus a) \oplus$

$a \neq \emptyset$. Moreover, one can easily check that $d \oplus (a \oplus z) \cap (d \oplus a) \oplus z \neq \emptyset$ and that $d \oplus (y \oplus a) \cap (d \oplus y) \oplus a \neq \emptyset$. If $y \neq a$ and $z \neq a$ then $d \in d \oplus (y \oplus z) \cap (d \oplus y) \oplus z$.

Remark 5. Every element in $(H,\oplus)$ is idempotent. This is trivial from chemical point of view as no reaction exists in an electrochemical cell between two identical elements, so, the element is unchanged.

Proposition 4. $(H,\oplus)$ is not a quasi-hypergroup nor a semihyperegroup.

Proof. Since d is not an element in $a \oplus H$, it follows that $(H,\oplus)$ is not a quasi-hypergroup. Having $a \oplus (d \oplus d) = \{b, c\} \neq (a \oplus d) \oplus d = \{b, c\} \oplus d = \{b, c, d\}$ implies that $(H,\oplus)$ is not a semihypergroup.

Proposition 5. $(H,\oplus)$ does not admit an identity element.

Proof. Since a, b, c, d are not elements of $a \oplus d, b \oplus c, c \oplus b, d \oplus a$, it follows that none of our elements is an identity.

Remark 6. Proposition 5 implies that there exists no element x in H (in a Galvanic/Electrolytic cell) such that the following reaction occurs for all y in H and some z in H:

$$x + y \rightarrow y + z.$$

Remark 7. Remark 2, Theorem 2 and Proposition 5 imply that $(H,\oplus)$ is not isomorphic to $(H,\oplus_1)$ nor to $(H,\oplus_2)$.

Proposition 6. There are only two H_v-subsemigroups of $(H,\oplus)$ up to isomorphism.

Proof. It is easy to see that $(\{a\},\oplus)$ and $(\{a, b\},\oplus)$ are the only H_v-subsemigroups of $(H,\oplus)$ up to isomorphism. Moreover, $(\{a\},\oplus)$ and $(\{a, b\},\oplus)$ are hypergroups.

Definition 7. Let $(H,\circ)$ be an H_v-semigroup and A be a non-empty subset of H. A is a complete part of H if for any natural number n and for all hyperproducts $P \in H_H(n)$, the following implication holds:

$$A \cap P \neq \emptyset \rightarrow P \subseteq A.$$

Proposition 8. $(H,\oplus)$ has no proper complete parts.

Proof. Let $A \neq \emptyset$ be a complete part of $(H,\oplus)$. We consider the following cases for A:

- Case $a \in A$. Having $a \in a \oplus x$, $x \in a \oplus x$ for all $x \in \{a,b,c\}$ imply that $x \in a \oplus x \subseteq A$. We get now that $b \in A$. Since $b \in b \oplus d$ and $d \in b \oplus d$, it follows that $d \in b \oplus d \subseteq A$. Thus, $A = H$.
- Case $b \in A$. Having $b \in b \oplus a$ implies that $a \in b \oplus a \subseteq A$. The latter implies that $a \in A$ and thus $A = H$ by the first case.
- Case $c \in A$. Having $c \in c \oplus a$ implies that $a \in c \oplus a \subseteq A$. The latter implies that $a \in A$ and thus $A = H$ by the first case.
- Case $d \in A$. Having $d \in c \oplus d$ implies that $c \in c \oplus d \subseteq A$. The latter implies that $c \in A$ and thus $A = H$ by the previous case.

Therefore, $(H,\oplus)$ has no proper complete part.

The main tools connecting the class of hyperstructures with the classical algebraic structures are the fundamental relations. The fundamental relation has an important role in the study of semihypergroups and especially of hypergroups.

Definition 9. For all $n > 1$, we define the relation β_n on an H_v-semigroup $(H,\circ)$ as follows:

$$x\beta_n\, y \text{ if there exist } a_1,\cdots,a_n \in H \text{ such that } \{x,y\} \subseteq \prod_{i=1}^{n} a_i.$$

and we set $\beta = \bigcup_{n\geq 1} \beta_n$, where $\beta_1 = \{(x,x) \mid x \in H\}$ is the diagonal relation on H.

This relation was introduced by Koskas [13] and studied mainly by Corsini [4], Davvaz [9], Davvaz and Leoreanu-Fotea [11], Freni [12], Vougiouklis [15], and many others. Clearly, the relation β is reflexive and symmetric. Denote by β^* the transitive closure of β.

The $\beta^*$is called the *fundamental equivalence relation* on H and it is the smallest strongly regular relation on H. If H is a hypergroup then $\beta = \beta^*$ [12] and H/β^* is called the *fundamental group*.

Proposition 10. $(H,\oplus)$ has a trivial fundamental group.

Proof. Since $\{a,b\} \subseteq a \oplus b$, it follows that $a\beta_2\, b$. Similarly, we obtain $a\beta_2$ c, $b\beta_2 d$, $c\beta_2 d$. Having β^* the transitive closure of β, one can easily see that $x\beta^* y$ for all $(x,y) \in H^2$. Thus, $|H/\beta^*| = 1$.

4. CONCLUSION

This paper provided a new chemical hyperstructure on electrochemical cells that is not equivalent to any of the studied chemical hyperstructures before.

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ABSTRACTS
IN
PERSIAN

Hypercube Related Polytopes

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ابرمکعب مربوط به چندبرها

ادیتور رابط: علیرضا اشرفی

چکیده

ساختارهای مرکز بدن، به عنوان بذرهایی برای انواع ساختارهای رتبهٔ 3 و بالاتر، مورد استفاده قرار گرفته‌اند. در این مقاله، ساختارهای رمبلن معرفی شده‌اند و طراحی و ویژگی‌های توپولوژیکی آنها به تفصیل بیان شده است.

لغات کلیدی: چندوجهی، n- چندبر، 24-سلول، رمبلن، رتبه

General Theory of Cycle–Dependence of Total π–Electron Energy

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نظریهٔ عمومی وابستگی چرخهٔ انرژی کل π-الکترون

ادیتور رابط : علیرضا اشرفی

چکیده

رفتار نظری اثرات چرخه روی انرژی کل π- الکترون که بطور عمده توسط تریناجستیک و گروه تحقیقاتی‌اش به دقت شرح داده شده است، مجددا در یک حالت کلی و رسمی‌تر بیان شده است. همچنین این موضوع به چندین روش ممکن برای اندازه‌گیری اثرات چرخه کمک کرده و به مسیرهای دیگری از تحقیق اشاره می‌کند.

لغات کلیدی: انرژی کلπ- الکترون، انرژی رزونانس توپولوژیکی، اثر انرژی چرخه، معطربودن، قضیهٔ ساچز

More Inequalities for Laplacian Indices by Way of Majorization

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نامساوی‌های بیشتر برای شاخص‌های لاپلاس به روش بیشینه‌سازی

ادیتور رابط : علیرضا اشرفی

چکیده

n- تایی مقادیر مشخصهٔ لاپلاس یک گراف، توسط دنبالهٔ مزدوج درجاتش بیشینه شده است. با استفاده از نتایج به دست آمده، مجموعه‌ای از نامساوی‌های عمومی را برای تعدادی از شاخص‌های لاپلاس بیان شده بر حسب درجات مزدوج، می‌یابیم و سپس با یک پارامتر ماکسیمال، کرانهای کلی مقید که بر حسب اندازهٔ مجموعهٔ رئوس n و درجهٔ میانگین $d_G=2|E|/n$ بیان شده‌اند را به‌دست می‌آوریم. همچنین تعدادی کران مقید مشخص برای تعدادی از کلاسهای گرافها برحسب پارامترهای گراف متعارف می‌یابیم.

لغات کلیدی: شاخص‌های لاپلاس، دنبالهٔ مزدوج، بیشینه‌سازی

Fractal-Like Kinetics Study of Adsorption on Multi-Walled Carbon Nanotube

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مطالعهٔ سینتیک فرکتالی جذب سطحی بر روی نانولولهٔ کربنی چنددیواره

ادیتور رابط : علیرضا اشرفی

چکیده

درجهٔ فرکتالی جذب بر روی سطح نانولوله‌های کربنی بررسی شده است. مدل سینتیکی لانگمویر فرکتالی برای بدست آوردن درجهٔ فرکتالی جذب یون بر روی نانولوله کربنی استفاده شده است. رفتار این معادله سینتیکی با برخی معادلات سرعت مثل لانگمویر، شبه مرتبه یک و شبه مرتبه دو مقایسه شده است. نشان داده شد که سینتیک جذب بر روی نانولوله می‌تواند برای بدست‌آوردن بعد طیفی ماده با موفقیت مورد استفاده قرار گیرد.

لغات کلیدی: نانو لوله کربنی چند دیواره، بعد طیفی، مدل لانگمویر فرکتالی، معادلهٔ سینتیکی، جذب سطحی

On Common Neighborhood Graphs II

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گراف‌های همسایه مشترک 2

ادیتور رابط : تومسیلاو داسلیک

چکیده

فرض کنید G یک گراف ساده با مجموعهٔ رئوس $V(G)$ است. گراف همسایه مشترک از G که با $con(G)$ نشان داده می‌شود، یک گراف با مجموعهٔ رئوس $V(G)$ است که در آن، دو رأس مجاورند اگر و فقط اگر حداقل یک همسایه مشترک در G داشته باشند. در این مقاله، ما گراف همسایه مشترک تعدادی گراف‌های مرکب را محاسبه می‌کنیم. با استفاده از این نتایج، همسایه مشترک چندین گراف خاص مشخص می‌شوند.

لغات کلیدی: گراف همسایه مشترک، گراف میسیلسکی، گراف شادو، گراف هجوس.

On the Eccentric Connectivity Index of Unicyclic Graphs

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شاخص اتصال خارج از مرکز گراف‌های تک‌دوری

ادیتور رابط : علیرضا اشرفی

چکیده

در این مقاله، کران های بالایی و پایینی شاخص اتصال خارج از مرکز گراف‌های تک‌دوری با تطابق کامل را به‌دست می‌آوریم. همچنین تعدادی کران پایین روی شاخص اتصال خارج از مرکز گراف‌های تک‌دوری با ارقام تطبیق داده شده را ارائه می‌کنیم.

لغات کلیدی: گراف تک‌دوری، شاخص اتصال خارج از مرکز، عدد تطبیق، تطبیق کامل

A Note on Revised Szeged Index of Graph Operations

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یادداشتی در مورد شاخص سگد بازنگری‌شده از عملگرهای گراف

ادیتور رابط : حسن یوسفی آذری

چکیده

فرض کنید G گرافی متناهی و ساده با مجموعه یال‌های $E(G)$ باشد. شاخص سگد بازنگری‌شده به‌صورت زیر تعریف می‌شود:

$$Sz^*(G)=\sum_{e=uv\in E(G)}\left(n_u(e\,|\,G)+\frac{n_G(e)}{2}\right)\left(n_v(e\,|\,G)+\frac{n_G(e)}{2}\right)$$

که $n_u(e|G)$ تعداد رئوسی در G است که به u نزدیکتر از v هستند و $n_G(e)$ تعداد رئوس هم‌فاصله از e در G است. در این مقاله، شاخص سگد بازنگری‌شده را برای عملگرهای اتصال و ضرب کرونا در گراف‌ها بررسی می‌کنیم.

لغات کلیدی: شاخص توپولوژیک، شاخص سگد بازنگری شده، عملگر گراف

Weak Chemical Hyperstructures Associated to Electrochemical Cells

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ابرساختارهای شیمیایی ضعیف مرتبط با سلول‌های الکتروشیمیایی

ادیتور رابط : ایوان گوتمن

چکیده

ابرساختارهای جبری کاربردهای زیادی در علوم مختلف دارند. هدف اصلی این مقاله، فراهم‌کردن کاربرد جدیدی از فراساختارهای ضعیف در شیمی است. بطور دقیق‌تر، سه نمونهٔ مختلف از ابراساختارهای مرتبط با سلول‌های الکترو–شیمیایی را ارائه می‌کنیم. ثابت می‌کنیم که ابرساختار های موردنظر، H_v- نیم‌گروه تشکیل داده و ویژگی‌های جالبی از آن‌ها را ارائه می‌کنیم.

لغات کلیدی: H_v- نیم‌گروه، بخش کامل، رابطهٔ اساسی، سلول گالوانیکی، سلول الکترولیتی

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