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Rhombellanic Crystals and Quasicrystals

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ABSTRACT

Design of some crystal and quasicrystal networks, based on rhombellane tiling, is presented. [1,1,1]Propellane, is a synthesized organic molecule; its hydrogenated form, the bicyclo[1.1.1]pentane, may be represented by the complete bipartite graph $K_{2,3}$ which is the smallest rhombellane. Topology of translational and radial structures involving rhombellanes is described in terms of vertex symbol, connectivity sequence, ring sequence and map operations relating structures to their seeds. It is shown, by alternating sum of ranked substructures, that radial structures represent complex constructions of higher rank. Basic properties of rhombellanes, coloring included, are outlined.

1 INTRODUCTION

[1,1,1]Propellaneis an organic molecule, first synthesized by Wiberg and Walker in 1982 [1]. By IUPAC rules, it is named Tricyclo[1.1.1.0^{1,3}]pentane, a hydrocarbon with formula C_5H_6 and three rings of three atoms. The hydrogenated form of propellane, C_5H_8, eventually named bicyclo[1.1.1]pentane, has only rhomb/square rings; it can be represented by $K_{2,3}$ - the complete bipartite graph, which is the smallest rhombellane. The two bridge carbon atoms can be functionalized, e.g., by bromine or COOH, or even by repeating the $K_{2,3}$ motif, as in the polymer called staffane [2].

Rhombic polyhedra are known as aesthetic appeal objects, of mathematical interest [3]; the well-known triacontahedron, the dual of Archimedean

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icosidodecahedron, has 30 rhombic faces. In the book “Multi-shell polyhedral clusters” [4],the cluster C_{152} was described consisting of $K_{2,3}$ units, which are not polyhedra cf. Steinitz Theorem [5] but tiles [6].

Design of rhombellanes is made by a general procedure [7], achieved as follows: join by a point (called “rbl-point”) the two vertices lying opposite diagonal in each rhomb of an all rhomb-map (i.e. 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, taking 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.

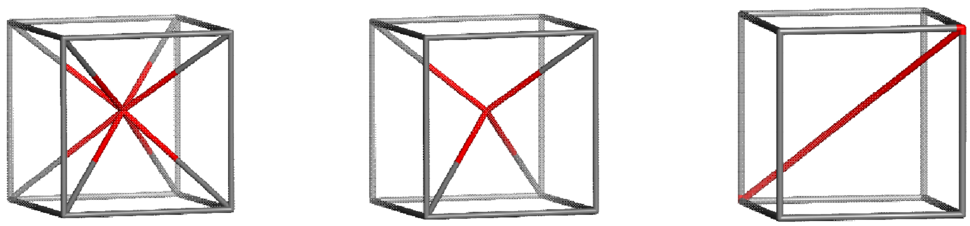
The paper is organized as follows: after an introduction, construction of some periodic rhombellane-consisting structures is presented; in the third section, non-periodic radial structures are discussed; the forth section details the rhombellanic character, in mathematical chemistry terms; in the fifth section, a graph coloring problem related to rhombellanes is exposed; conclusions and references will close the paper.

2. PERIODIC RHOMBELLANIC STRUCTURES

According to Steinhardt definition [8], crystals are highly ordered structures, with atomic clusters repeated periodically, in three independent directions of the space, and showing an essentially discrete diffraction diagram; the symmetry of infinite crystal lattices is completely described by the 230 symmetry groups of the space.

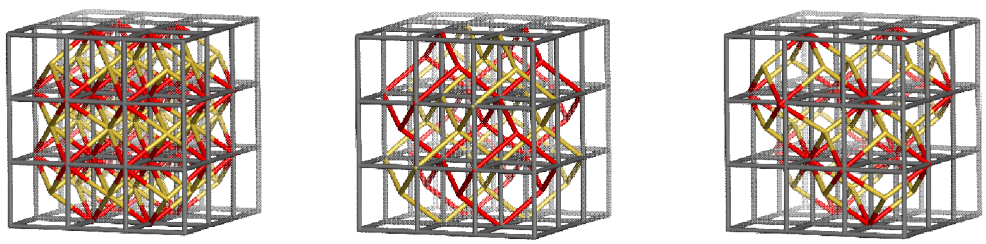
Starting from the simplest crystal network, namely the simple cubic *pcu* net, of which repeating unit is a cube C, it is possible to build a variety of triple periodic structures.

Let first locate a point/atom in the center of cube and join it with all the corners of cube; the obtained unit is referred here as $CP^8.9$ (Figure 1, left), P^8 meaning a point of connectivity 8. By translating this unit along the three coordinate axes results in a “body centered cubic” *bcc* network, including both *pcu* and *bcu* networks; by this reason, it is named here *pcu-bcu* (Figure 2, left). Second, cut-off, in an alternating manner, four of the edges emerging from the central point to the corners of cube; the unit thus obtained is named $CP^4.9$ (Figure 1, middle) while the network resulted from itby a simple translation is denoted *pcu-dia* (Figure 2, middle). Third, translate CP^4 unit along the three coordinate axes, each step rotated 90^o, thus resulting the network called here *pcu-flu* (Figure 2, right); its repeating unit consists of eight CP^4 units, with a total of 35 points/atoms.



$CP^8.9$ (*pcu-bcu*) $CP^4.9$ (*pcu-dia*); (*pcu-flu*) CD.8 (*bcu*)

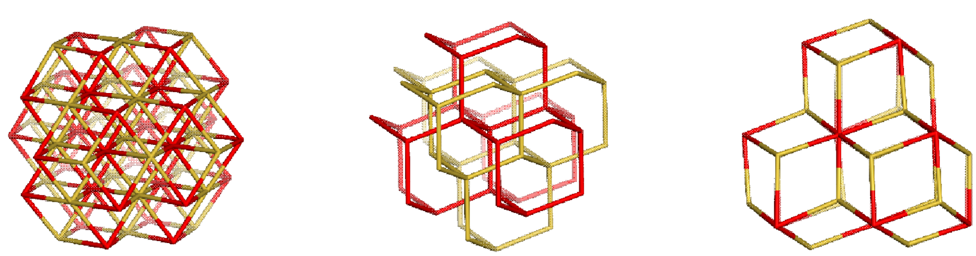
Figure 1. Seeds for three periodic networks.



pcu-bcu $CP^8.9$ *pcu-dia* $CP^4.9$ *pcu-flu* CP^4& $CP^4R(90^o)$

Figure 2. Networks superposed over the simple cubic net *pcu*; seeds are indicated on the bottom row.

The *bcu*, *dia* and *flu* nets alone (see [9] for symbols), resulted by deleting the *pcu* net (Figure 2), are illustrated in Figure 3. Also, *bcu* can be generated by translating the unit CD.8 (Figure 1, right), a diagonalized cube, representing a substructure of the unit $Rh_{12}P^8.15$ (Figure 4, top, middle).



bcu (*Im-3m*) *dia* (*Fd-3m*) *flu* (*Fm-3m*)

Figure 3. Periodic nets envisaged by deleting the simple cubic net *pcu* in Figure 2.

The void of *flu* net is the rhombic dodecahedron $Rh_{12}.14$ (Figure 4, top, left), a space filler. By doping Rh_{12} with a body centered atom, P^8, results in $Rh_{12}P^8.15$, a cluster of rank $k = 5$ (see Table 1S, Supplementary material); it is the seed of *bcu* net (Figure 5, top, middle and right); relation between the two netsorks is illustrated in Figure 4.Any atom of *bcu*is retrievedin the *pcu* (*i.e.*, twin/entangled *pcu*) net (and the reciprocal is true); it is clear that Figure 2, left, shows the *bcu* net with the rectangular edges of *pcu* also represented. However, any of *flu* atoms belongs to the (twin) *pcu* but the reciprocal is not true.

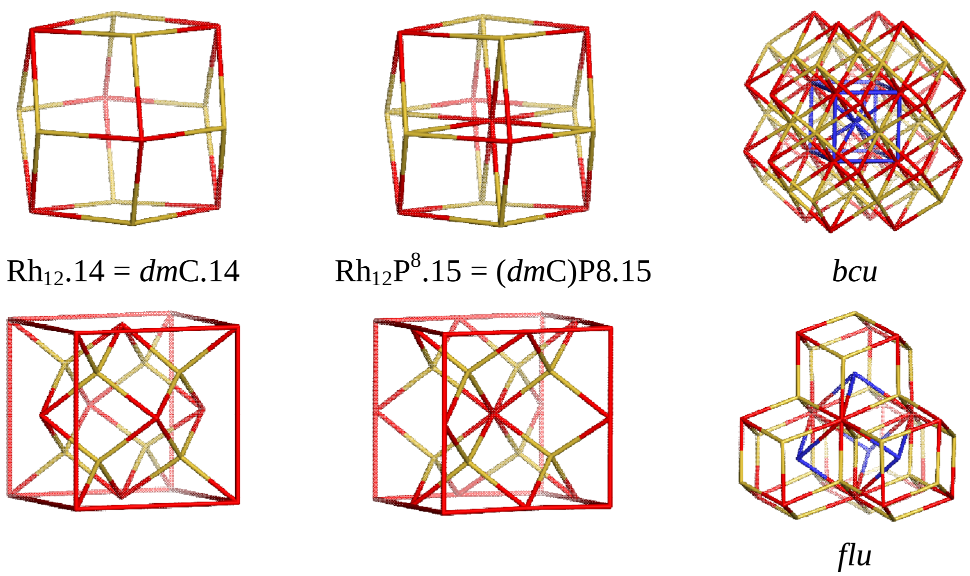
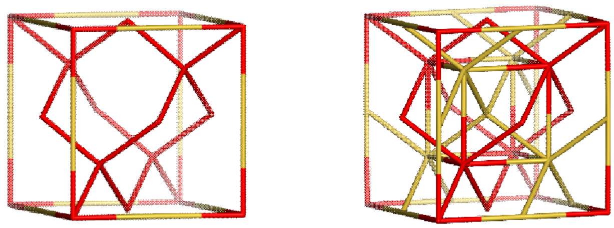


Figure 4. Doping by a point/atom the seed of *flu*, Rh_{12} (top, left), becomes $Rh_{12}P^8.15$ (top, middle), the seed of *bcu* (top right); the void Rh_{12} and its complement (within the *pcu* frame) form the *flu* net (bottom).

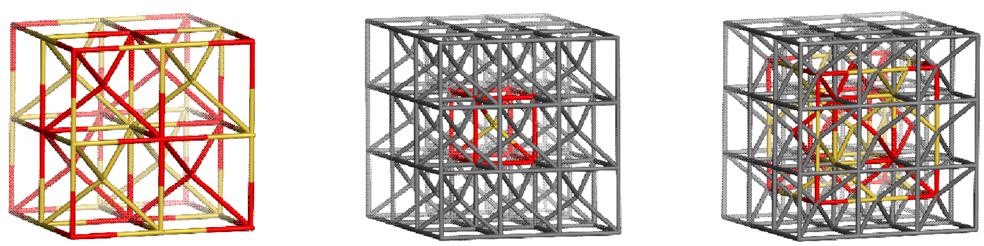
Similarly, the net *pcu-dia* (Figure 2, middle), of which seed is $CP^4.9$, is in fact the twin *dia* net, of *Fm-3m* space group: a “face centered cubic” *fcc* net is entangled with its self-dual net; the two nets are displaced along the body diagonal of the cube by one quorter of the diagonal length, as illustrated in Figure 5. Any atom of (twin) *dia* is retrieved in the (twin) *pcu* net (and the reciprocal is true); in the retrieved *pcu* net, the atoms of the two *dia* nets alternate in populating the cubic net, as in the cube bipartite coloring (Figure 6). If rotates 90^o to each other (and identifies the superposed points) *dia-dia* changes to the *flu* net (Figures 3 and 4).

Triple periodic networks can be characterized by sequences of vertex connectivity, as given in the crystallographic databases [9]. Sequences of a given topological property are counted as rows in layer/shell matrices, LM/ShM [10,11]; in this case, LC is the layer of connectivity matrix, which is taken up to the distance ten from the chosen vertex. In addition, if the strong rings surrounding vertices are considered, the layer of rings matrix LR [12] can be obtained; the characterization of a triple periodic network is (for the first time) more complete. Lists of such data for the nets: *pcu*, *bcu*, *fcu*, *dia*, *flu*, *pcu-bcu*, *pcu-dia* and *pcu-flu* are given elsewhere (Tables 2S and 3S – Supplementary material). (The figure count for the seeds of the discussed networks is given in Table 1S– Supplementary material).



ada = dia_{fcc} *dia* (*Fd-3m*) co-*ada* = dia_{bcc}

Figure 5. Diamond net substructures entangled within the *pcu* frame: *dia* = ∪(*fcc*; *bcc*).

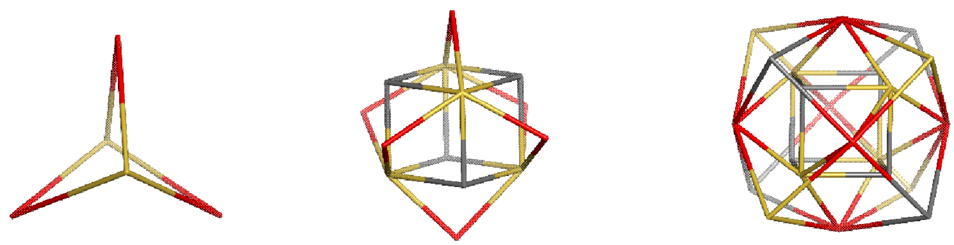


ada = dia_{fcc} Cubic *dia* Twin *dia* (entangled)

Figure 6. Two *dia*-nets complementarily occupy the same space generated by the CP^4 seed: there is only one *ada* unit (red) and one co-*ada* (yellow – left); in the cubic *dia* net, the space filler is only CP^4 unit (red – middle); in the retrieved *pcu* net, the atoms of the two entangled *dia* nets alternatively populate the cubic net, as in the bipartite coloring (right).

3. RHOMBELLANIC RADIAL STRUCTURES

Quasicrystals are finite aperiodic structures, with long-range positional and orientational order [8]. Among the rotational symmetries, 2−, 3−, 4− and 6−fold axes are allowed in crystals, while 5−, 7− and all higher (non-crystallographic) rotational symmetries are encountered in quasicrystals. Atomic clusters are repeated in a complex, non-periodic pattern; electron diffraction shows sharp patterns, as found experimentally by Shehtman [13] the Nobel prize winner in 2011. Radial structures with rhombellanic characteristics can be obtained by applying iteratively the "rhombellation" procedure, described in the introductory section. The procedure is illustrated in Figre 7, starting from the cube.



$Rh_3 = K_{2.3}$ Rh_6 and rbl points (in red) rbl_1 generation (Rh_{12} hull)

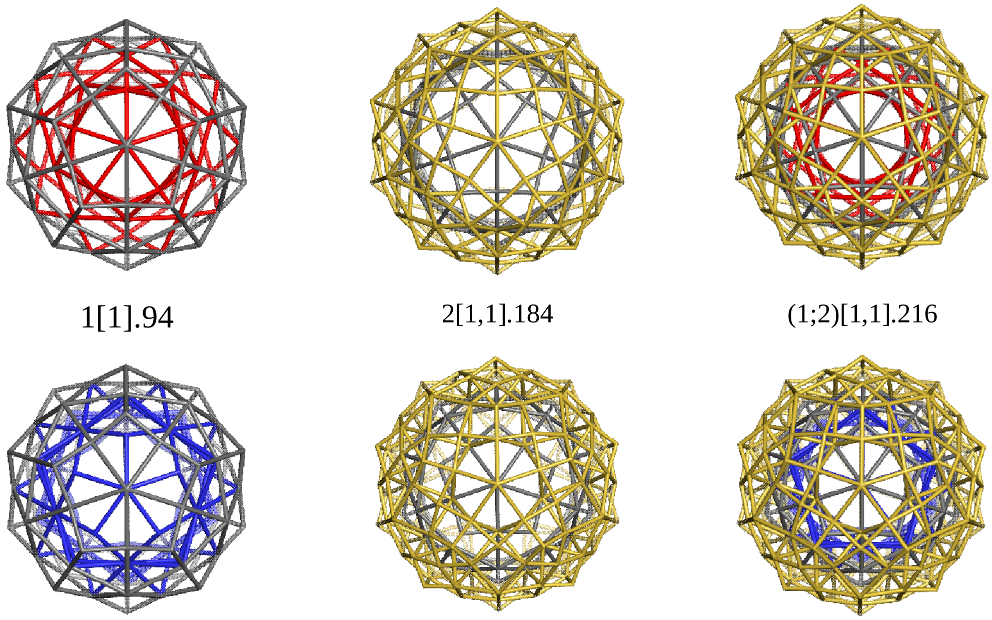
Figure 7. Rhombellane Rh_3 and rhombellation starting from the cube (*i.e.*,Rh_6).

The new envelope Rh_{n+1} has twice the number of rhombs in the precedent Rh_n envelope; the number of vertices in a new generation is counted iteratively as: $v_{n+1} = v_n + 2h_n + 2$, with $v = |V(G)|$ being the number of vertices, h_n the number of rhombs in the hull of n-generation (embedded in the sphere) and 2 is the Euler characteristic (see below) of the sphere. Referring to the zero-generation, Rh_0, the actual number of vertices can be obtained by the formula:

$$v_n = 2(n+1) + h_0\,(2^{n+1} - 1).$$

Radial series can be characterized, as the crystal structures, by shells of connectivity LM and shells of rings around vertex LR matrices (see Supplementary material, Table 4S).

About space dimensionality or ranking, as defined by Schulte [14], each rhombellane generation (*i.e.* shell) can be seen as a cluster of rank k = 4 (Table 1); then, two such shells share a common 3-facet, which is a sphere tessellated by rhombs f_4, a true cell (Figure 8). It means, a shell pair (1;2) or (2:3) are structures of rank k = 5. Further, a pair {(1;2);(2:3)} will share a shell of rank k = 4 (in this case, the shell (2)); thus, the structure 3_{full}, (Table 1, bottom), bonded by two facets of rank $k = 5$, is a structure of rank $k = 6$ and the process can continue.



1[1].94 | 2[1,1].184 | (1;2)[1,1].216

1[2].94 | 2[2,2].184 | (1;2)[2,2].216

Figure 8. Facets of the shell pair (1;2) of rhombellanes $rbl_n(Rh_{30})$.

Table 1. Figure count for $Rh_{30}rbl_n[1,..,1]$; $K_{2.3}^* = f_4/3$; M = No. (inner + outer) cells.

[1,..,1]	v	e	f_4	$K_{2.3}$	$K_{2.4}$	$K_{2.5}$	Rh_8	Rh_{10}	$K_{2.3}^*$	M	3	4	5	6
1	94	240	270	20	0	0	0	12	90	2	124	0	(30;60)	
2	184	480	540	20	0	12	30	0	180	2	244	0	(60;120)	
3	364	960	1080	20	30	12	60	0	360	2	484	0	(120;240)	
(1;2)	216	600	750	40	0	12	30	12	270	2	366	2	2	-
(2;3)	426	1200	1470	40	30	24	60	0	540	2	696	2	2	-
3_{full}	458	1320	1710	60	30	24	90	12	630	2	848	2	2	0

Note, in Table 1, the presence of $K_{2.n}$ complete bipartite graphs and related rhombic cells Rh_n; also note the count of f_4 (pair (Rh_n, Rh_{n+1}) at the top of #5 and #6 columns). For the series [2,..,2], see Table 5S, (Supplementary material). Euler characteristic χ [15] of a surface S can be calculated as an alternating sum of figures, of rank k: $\chi(S) = f_0 - f_1 + f_2 - f_3 + ...,$.

4. RHOMBELLANIC CHARACTER

Proposition [7]. *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.*

Cube (actually Rh_6) is an all-square graph and Hamiltonian; its line-graph, the cuboctahedron, is also Hamiltonian but its Omega polynomial [16,17]: Ω(C) = 3X^4, meaning not all of its edges are topologically parallel; also, the vertices of cube form a singlevertex class and thus cannot be disconnected.

Triacontahedron, Rh_{30}, has all-square rings, all non-connected vertex classes but not 1X^*e* Omega polynomial unique term and no Hamiltonian circuit of its lines. Rhomb Icosahedron, Rh_{20}, has not all classes of non-connected vertices.

Omega polynomial is defined as: $\Omega(x) = \Sigma_k m x^s$, *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: $\Omega(x) = 1x^s$; $s = e = |E(G)|$, in other words, "all the edges in *G* are topologically parallel". However, Hamiltonicity is an *NP* complete problem, being taken here as a corollary of a single *ops* in Omega polynomial; however, not all the graphs having a Hamiltonian circuit have all the edges topologically parallel (see the case of cube and cuboctahedron).

The smallest rhombellane Rh_3 is $K_{2.3}$, the complete bipartite graph (corresponding to the molecular graph of C_5H_8, bicyclo[1.1.1]pentane); all $K_{2.n}$ graphs fulfill all the above conditions. Any $K_{2.n}$ graph consists of $n(n-1)(n-2)/6$ $K_{2.3}$ substructures. There are rhomb-tessellated cages that fulfil the first four criteria but do not contain any $K_{2.3}$ substructure.

Further, there are graphs with more than two vertex classes obeying the above conditions. Rhombellation operation provides such graphs, with *n* shells/generations, when applied iteratively. The rbl-vertices added in the first step of any new generation are disjoint with respect to each other while in the second step they are joined by means of new vertices superposed on the parent vertices (thus not connected, neither to the parent vertices nor to themselves); this construction provides classes of vertices non-connected to each other within a same class. Rhombellanes represent *n*-partite graphs, both by topology and coloring (see below). Rhombellanic crystal networks also fulfill all the five above criteria: among the discussed network, only the *dia* net (as the superposed *pcu-dia*) is full rhombellanic, whereas *pcu-bcu* has triangles while *flu* does not cover all points/atoms in *pcu*. Accordingly, only the $CP^4.9$ seed show a full rhombellanic character.

Corollary. *In a finite molecular rhombellane, with vertex classes consisting of distinct atom types, there are only polar bonds while covalent non-polar bonds may not exist.*

5. Coloring Problem

The chromatic number *Ch* of a graph is the smallest number of colors needed to color its vertices so that no edge has the both endpoints colored the same [18]. Several graph constructions have been proposed about graph coloring [19−22]; two of them are more related to our proposed construction:

Mycielski's Theorem ([23], 1955). For any integer $n > 1$, there exists a triangle-free n-chromatic graph.

Zykov's Theorem ([24], 1949): There exist triangle-free graphs with arbitrary large chromatic number.

Hamiltonicity and other properties of triangle-free graphs transformed by Mycielski's construction were discussed in [25,26]. Note that, the 4-polytope 24-Cell is three-colored, its medial (i.e., line-graph) C_{96} is four-colored, its face-dual is also four-colored; however, these graphs have a single topological vertex class; it means, the coloring does not superposes over topology. Also, bipartite graphs (i.e. graphs with all even size cycles) have $Ch = 2$ but may have more than two topological vertex classes. In rhombellanes, topology superposes over coloring; for $rbl_1(C).22$, we found $Ch = 5$; for $rbl_2(C).48$, $Ch = 8$.

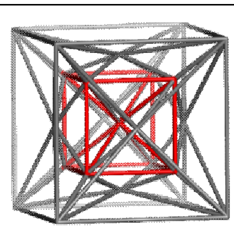
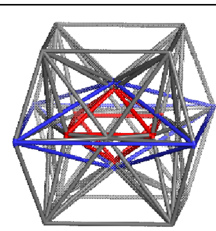
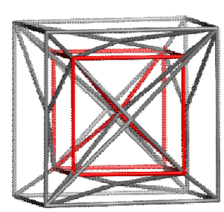
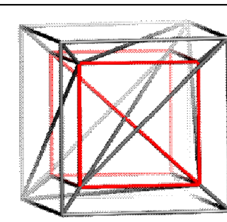
			
$Q_4.8CP^8.24$ = 24-Cell Ch=3, Cls=1	$Q_4.8CP^8.24$ Torus $T_{4,4}$ embedding	$Q_4.8CP^4sa.24$ Ch=2, Cls=2	$Q_4.CD.16$ Ch=16, Cls=16

Figure 9. Hypercube Q_4 derivatives.

Jensen and Royle [27] provided an easy construction of a 22-vertex graph (from the Grötzsch graph) and an easy proof that the result is triangle-free and 5-chromatic. By repeating two times Mycielski's procedure, a 45-vertex, triangle-free, 6-chromatic graph was obtained; it is unknown if a smaller such graph exists [18] (however, graphs of 44 or 43 vertices were questioned [28]). In this light, our results are correct, with respect to chromatic number and our procedure seems to be simpler than those already published.

Rhombellation operation provides triangle-free graphs with arbitrarily large chromatic number. Figure 9 illustrates three derivatives of the hypercube Q_4 – Tesseract, in four representations: (i) $Q_4.8CP^8.24$=24-Cell (Ch=3; Cls=1); the construction is made in the idea of cube-derivatives CP^8, CP^4 and CD, used as network seeds (Figure 1) and seems to be a new way to build the 24-Cell 4-polytope [7]; it has $Ch = 3$ but is not rbl in character (it contains triangles and has a single class of vertices, thus cannot be disconnected); (ii) The object $Q_4.8CP^8.24$ embedded in the torus $T_{4,4}$;(iii) $Q_4.8CP^4sa.24$, a syn-anti isomer with $Ch = 2$ and Cls=2; it has a rbl character and (iv) Q_4.CD.16, a diagonalized hypercube having $Ch=|V(G)|=16$ (i.e., the number of atoms/vertices in the molecule/graph); in other words, each class consists of singular vertices, clearly disconnected, as they belong each to different classes; this is also a rhombellanic structure, obeying all the five rbl criteria. Topology of these Q_4-derivatives is given in Tables 6S to 8S (Supplementary material).

Vertex classes were computed by our Nano-Studio software [29], as centrality indices, and confirmed by permutations in the adjacency matrix of graphs, performed by Mathematica [30].

6. CONCLUSIONS

Rhombellane, Rh_3 or $K_{2.3}$, is the smallest tile with rhombic rings/faces; it represents a real chemical molecule. Generalized rhombellanes, designed by the rhombellation procedure, have non-connected vertex classes (of interest in graph coloring); all the edges are topologically parallel (as shown by the single term Omega polynomial, further involving Hamiltonian circuits visiting their edges) and contain at least one $K_{2.3}$ subgraph.

For some well-known triple periodic crystal networks, like *pcu*, *bcu* or *dia*, rhombellanes enable a deeper description, helpful in understanding relations among networks apparently not related. Cube-like molecules or crystal networks have been reported [31,32]. For the first time in literature, crystals and quasicrystals were characterized by sequences of strong rings around atoms.

Exploring network seeds led to a new building way of the 4-polytope 24-cell. Radial structures, generated by propellation are ordered (yet hypothetical) structures of higher rank.

Rhombellanes represent a new class of structures, with promising properties, both in theory and applications.

Supplementary Material. Available on request, at www.esmc.ro.

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One–Alpha Descriptor

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ABSTRACT

Recently, one-two descriptor has been defined and it has been shown that it is a good predictor of the heat capacity at *P* constant (CP) and of the total surface area (TSA). In this paper, we analyze its generalizations by replacing the value 2 by arbitrary positive value α. We show that these analyses may be on interest, because even good predictions of CP and TSA can be slightly improved. Furthermore, it can be expected that this more general descriptor can find a wider range of application than the original one. The extremal values of trees have been found for all values of α.

1 INTRODUCTION

The molecular descriptor is the final result of a logical and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment [2]. Molecular descriptors have been shown to be useful in modeling many physico-chemical properties in numerous QSAR and QSPR studies [3-5].

In this paper, we introduce one-alpha descriptor. It is defined as the sum of the vertex contributions is such a way that each pendent vertex contributes 1, each vertex of degree two adjacent to pendent vertex contributes α, and also each vertex of degree higher than two also contributes α and another vertex contributes 0. If we take α=2, we get the previously defined [1] one-two descriptor. As in [1], we illustrate this definition for 3-ethyl-hexane in Figure 1.

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One-alpha descriptor of graph G will be denoted by OA(G). For instance, if G is 3-ethyl-hexane, then OA(G) = 3 + 4α. We show that one-alpha descriptor as generalization of one-two descriptor may be of interest in chemistry, since it can slightly improve predictions of the heat capacity at *P* constant (CP) and of the total surface area (TSA) for octane isomers. Further, we analyze mathematical properties of this descriptor. Namely, we find tight upper and lower bounds in the families of the trees with n vertices and the chemical trees with n vertices.

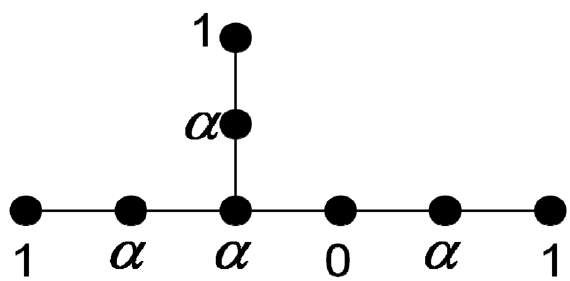

Figure 1. Vertex contributions of 3-ethyl-hexane. Each pendent vertex contributes 1, each vertex of degree two adjacent to pendent vertex contributes α, and also each vertex of degree higher than two also contributes α and another vertex contributes 0.

2. QSAR RESULTS

International Academy of Mathematical Chemistry [6] proposed four benchmark sets [7] as sets for testing the molecular descriptors. Also, recently Adriatic descriptors [8−12] have been proposed and in many cases they have provided better results than benchmark descriptors [8,11]. One-two descriptor outperformed both sets of descriptors in the linear modeling of TSA, and it was of comparable quality (slightly better) than benchmark descriptors in the linear modeling of CP, but not as good as the best Adriatic index [8−12].

However, here we show that α =2 does not give the best results in the set of all one-alpha descriptors. Namely in the linear modeling of TSA, the best results are obtained for α ≈1.8 and in the linear modeling of CP, the best results are obtained for α ≈ 2.18. The histograms that illustrate the changes of r^2 in the dependence of the values of α are presented on the Figures 2 and 3:

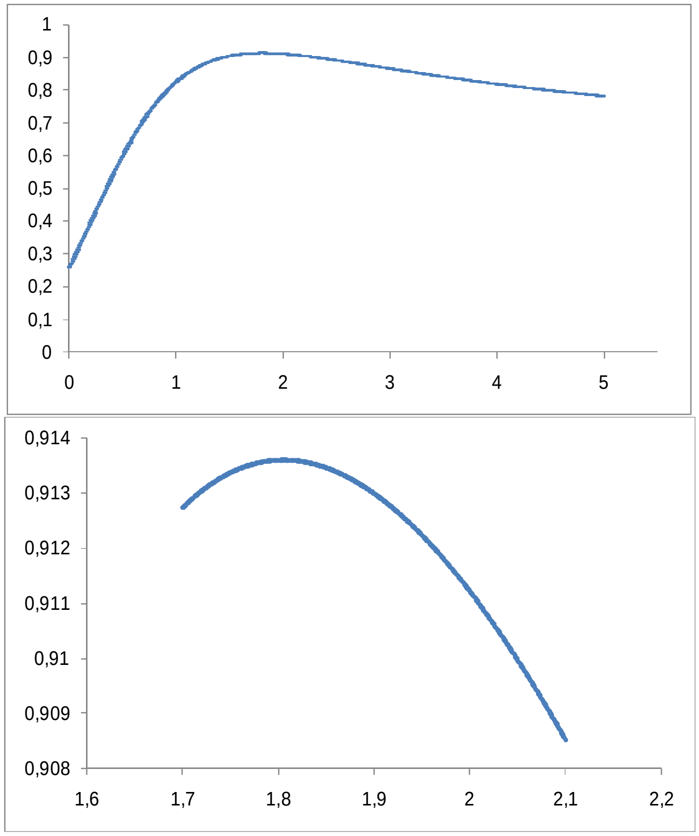

Figure 2. r^2 values of the linear models for estimation of the total surface area by one-alpha descriptors. On the left hand-side diagram α ∈ [0,5] and on the right hand-side diagram α ∈ [1.7, 2.1].

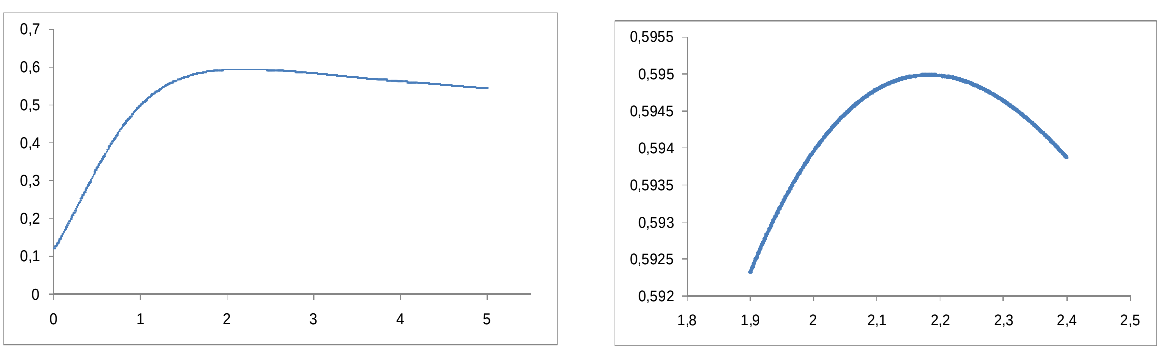

Figure 3. r^2 values of the linear models for estimation of the heat capacity at P constant by one-alpha descriptors. On the left hand-side diagram α ∈ [0,5] and on the right hand-side diagram α ∈ [1.9, 2.4].

3. MATHEMATICAL PROPERTIES

Before proving the main theorems, let us introduce some notations. By $n_i(G)$ we denote the number of vertices of degree i in G and by $d_G(u)$ we denote the degree of vertex u in graph G. Let x be any real number. By [x] we denote the greatest integer not greater than x. In the proofs of the main theorems, we shall use the following well known lemmas:

Lemma 1. Let G be a tree with at least 2 vertices. Then it holds:

$$n_1(G) = \sum_{i\geq 3}(i-2)\,n_i(G) + 2\,.$$

Proof. It is easy to see that:

$$\begin{aligned}\sum_{i\geq 3}(i-2)\,n_i(G)+2 &= \sum_{i\geq 3} i n_i(G) - 2\sum_{i\geq 3} n_i(G)+2\\ &= \big(2\,|V(G)| - n_1(G) - 2n_2(G) - 2\big)\\ &\quad - 2\big(|V(G)| - n_1(G) - n_2(G)\big) + 2\\ &= n_1(G).\end{aligned}$$

Lemma 2. Let G be a tree with maximal upper bound for one-alpha descriptor. Then G does not contain any vertices of contribution 0 to OA index.

Proof. Supposed to the contrary that there exists a vertex u of contribution 0, and adjacent to vertices v_1 and v_2 such that $d_G(v_1)$, $d_G(v_2) \geq 2$. Let $G' = G - uv_2 + v_1v_2$. It can be easily seen that contributions of all the vertices except u and v_1 to OA index remained the same, the contribution of v_1 did not decrease and the contribution of u increased from 0 to 1. Hence, $OA(G') > OA(G)$, which is contradiction. Hence, indeed there are no vertices of contribution 0. □

Lemma 3. Let G be a tree with maximal upper bound for one-alpha descriptor and $\alpha > 1$. Then G has at least a vertex of degree 2.

Proof. By Lemma 1,

$$n_1(G) = \sum_{i\geq 3}(i-2)\,n_i(G) + 2 \geq \sum_{i\geq 3} n_i(G) + 2\,.$$

By the above inequality we conclude that, $n_1(G) - 2 \geq \sum_{i\geq 3} n_i(G)$. By contrary we assume that $n_2(G) = 0$. Since $n_1(G) + \sum_{i\geq 3} n_i(G) = n$, $n_1(G) + n_1(G) - 2 \geq n_1(G) + \sum_{i\geq 3} n_i(G) = n$ and so $n_1(G) \geq n/2 + 1$, where $|V(G)| = n$.

Also, since $n_2(G) = 0$, $OA(G) = n_1(G) + \alpha\sum_{i\geq 3} n_i(G) = n_1(G) + \alpha(n - n_1(G))$. By assumption OA(G) is maximal and $\alpha > 1$, then $n_1(G)$ must have minimum value. Now we construct a graph G' such that $|V(G')| = n$ and $n_1(G) < n/2+1$ and $OA(G') > OA(G)$, which makes contradiction. There are three cases for $n \geq 4$, $n = 3k + 1$, $n = 3k + 2$ or $n = 3k + 3$.

For each case we construct the graph G' as Figure 4, such that $OA(G') = n_1(G') + \alpha(n-n_1(G'))$, $n_1(G') < n/2+1$ and $OA(G') > OA(G)$, which is contradiction. □

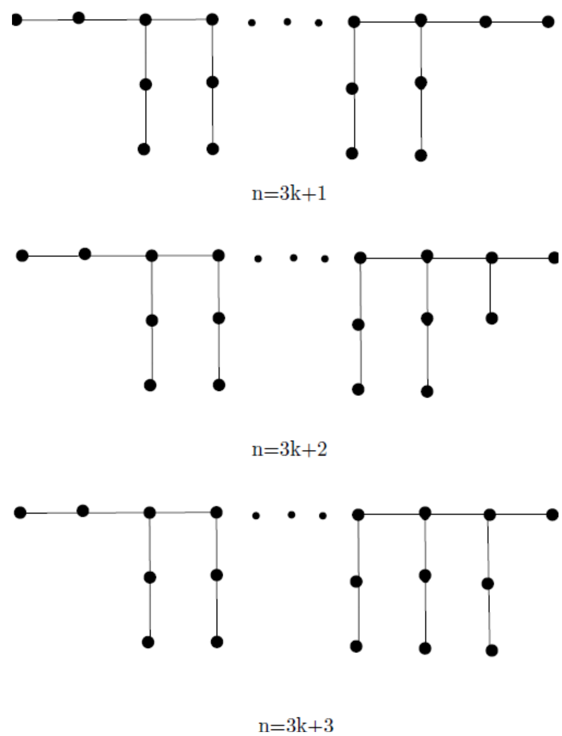

Figure 4. The constructed graph related Lemma 3.

Now, we can obtain lower and upper bounds for trees to different values of α.

Theorem 4. Let *G* be a tree with n vertices. It holds

$$OA(G) \geq \begin{cases} 0 & n=1 \\ 2 & n=2 \\ 2+\alpha & n=3 \\ \begin{cases} 2+2\alpha & \alpha < n-3 \\ 2n-4 & \alpha = n-3 \\ (n-1)+\alpha & \alpha > n-3 \end{cases} & n \geq 4 \end{cases}.$$

Proof. To prove the lower bound for OA(G), it can be easily checked for $n \leq 3$. For n=1, 2, 3 the lower bound can be obtained immediately. Hence, let us assume that $n \geq 4$. We use this well known fact that each tree with at least two vertices has at least two leaves. If G is a star, then it is easy to see that $OA(G) = (n-1) + \alpha$. If G is not a star, than there are at least two vertices adjacent to leaves hence $OA(G) \geq 2 + 2\alpha$. Now if $\alpha = n - 3$, then $2 + 2\alpha = (n-1) + \alpha = 2n - 4$ and hence for $\alpha < n-3$, we have $2 + 2\alpha < (n - 1) + \alpha$. Also for $\alpha > n - 3$, $2 + 2\alpha > (n - 1) + \alpha$. Examples of the extremal graphs obtaining the lower bounds for $\alpha < n - 3$ are paths P_n, for $n \geq 4$ and for $\alpha > n - 3$ are the stars S_n, for $n \geq 4$. Also for $\alpha = n - 3$, $OA(P_n) = OA(S_n) = 2n - 4$. □

Theorem 5. Let *G* be a tree with *n* vertices. Then

$$OA(G) \leq \begin{cases} (n-1)+\alpha & \alpha \leq 1 \\ \begin{cases} \frac{n+2}{3} + \alpha(n - \frac{n+2}{3}) & \alpha > 1,\ \frac{n+2}{3} \in Z \\ \left\lfloor \frac{n+2}{3} \right\rfloor + 1 + \alpha(n - \left\lfloor \frac{n+2}{3} \right\rfloor - 1) & \alpha > 1,\ \frac{n+2}{3} \notin Z \end{cases} \end{cases}.$$

Proof. First assume that $\alpha \leq 1$. By Lemma 2, $OA(G) = n_1(G) + \alpha(n - n_1(G))$, then $OA(G)$ is maximum if and only if $n_1(G)$ is maximum. A tree with maximum number of leaves is a star and $OA(S_n) = (n - 1) + \alpha$. Therefore, $OA(G) \leq (n - 1) + \alpha$.

Now we assume that $\alpha > 1$. Let us prove that for each n, there exists an n-vertices tree G with maximum OA such that $\Delta(G) \leq 3$. Suppose that G is a tree with n vertices such that $OA(G)$ is maximum. If $\Delta(G) \leq 3$, then there is nothing to prove. Let $\Delta(G) > 4$, by Lemma 3, there exists a vertex v in V(G) such that $\deg_G v = 2$. Let $u \in V(G)$, $\deg_G u = \Delta(G)$ and $T_1, T_2, \ldots, T_{\Delta(G)}$ be branches from u, see Figure 5. Without loss of generality, we can assume that v is in T_1.

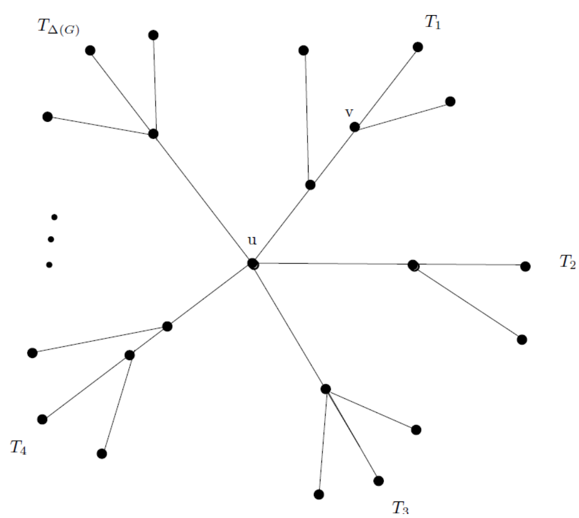

Figure 5. The configuration of graph G in Theorem 5.

Now we instruct a graph G_1 as follow: We omit the branches $T_4, T_5, \ldots, T_{\Delta(G)}$ and join them to vertex v. By this transformation we obtain the tree G_1, such that $OA(G_1)$ =

$OA(G)$ and since $OA(G)$ is maximum then $OA(G_1)$ will be maximum, then by Lemma 3 there exists a vertex v_1 in $V(G_1)$, such that $d_{G1}(v_1)=2$. It is clear that $\Delta(G_1) \leq \Delta(G)$ and $d_{G1}(v) = \Delta(G) - 1$. By continuing the above process we can obtain the graph G_2, such that $\Delta(G_2) \leq \Delta(G_1) \leq \Delta(G)$ and $OA(G_2) = OA(G_1) = OA(G)$. Finally by continuing this process we can obtain the graph G_s from G_{s-1}, such that $\Delta(G_s) \leq 3$ and $OA(G_s) = ... = OA(G_1) = OA(G)$. Hence from beginning we can assume that G is a tree with maximum OA and $\Delta(G) \leq 3$. Now by Lemma 1, $n_1(G) = \sum_{i\geq 3}(i - 2)\, n_i(G) + 2 = n_3(G) + 2$. We have $n_1(G) + n_2(G) + n_3(G) = 2$, and so

$$2\, n_1(G) + n_2(G) = n + 2. \tag{1}$$

By Lemma 2, G does not contain any vertices of contribution 0 to OA index then $OA(G) = n_1(G) + \alpha(n - n_1(G))$. Since $\alpha > 1$, $OA(G)$ is maximum if and only if $n_1(G)$ is minimum. Again, by Lemma 2, we have $n_2(G) \leq n_1(G)$. From Equation (1), we conclude that $3n_1(G) \geq 2n_1(G) + n_2(G) = n + 2$ and then $n_1(G) \geq (n + 2)/3$. Hence if

$$(n + 2)/3 = k \in Z \ (n \equiv 1 \bmod 3),$$

then $n_1(G)=(n+2)/3$ is minimum value for $n_1(G)$ and if

$$(n + 2)/3 = k \notin Z \ (n \equiv 0 \text{ or } 2 \bmod 3),$$

then $n_1(G)=[(n+2)/3]+1$ is minimum value. The examples of the extremal graphs obtaining the upper bounds are presented in the Figure 6.

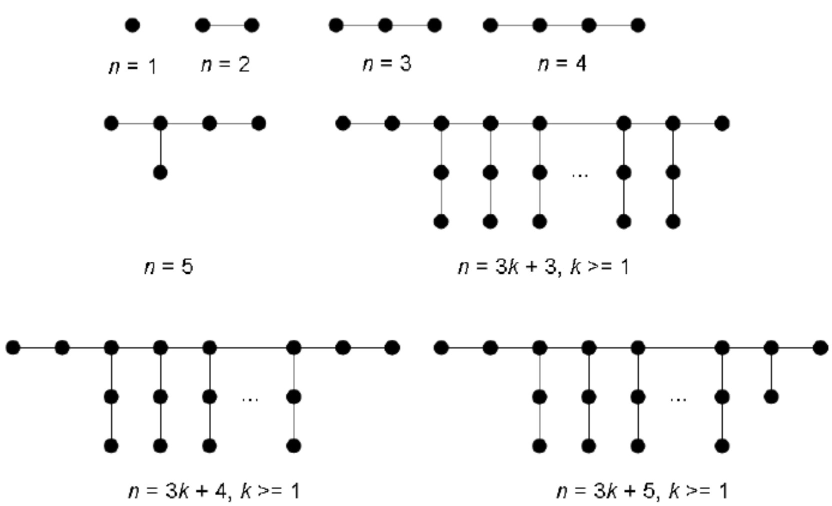

Figure 6. Extremal graphs obtaining the upper bounds.

This proves the Theorem. □

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A New Family of High-Order Difference Schemes for the Solution of Second Order Boundary Value Problems

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ABSTRACT

Many problems in chemistry, nanotechnology, biology, natural science, chemical physics and engineering are modeled by two point boundary value problems. In general, analytical solution of these problems does not exist. In this paper, we propose a new class of high-order accurate methods for solving special second order nonlinear two point boundary value problems. Local truncation errors of these methods are discussed. To illustrate the potential of the new methods, we apply them for solving some well-known problems, including Troesch's problem, Bratu's problem and certain singularly perturbed problem. Bratu's and Troech's problems, may be used to model some chemical reaction-diffusion and heat transfer processes. We also compare the results of this work with some existing results in the literature and show that the new methods are efficient and applicable.

1. INTRODUCTION

The study through boundary value problem is an interesting in recent years. This interest can be attributed due to its wide range of application in scientific research. In general, nonlinear boundary value problems do not always have solutions which we can obtain using analytical methods. Therefore, techniques for rapidly computing approximate solutions of boundary value problem are very importance.

In this paper, we introduce two fast and accurate numerical schemes for the solution of second-order nonlinear differential equations of the form

$$y'' = f(x, y), \qquad a < x < b, \tag{1}$$

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subject to the boundary conditions:

$$y(a) = \alpha, \qquad y(b) = \beta, \tag{2}$$

where a, b, α and β are the given constants. The existence and uniqueness of the solutions to problem (1)–(2) are discussed in [1]. The literature on the numerical approximation of solutions of boundary value problems is large and still growing rapidly. Among the most recent works concerned with numerical methods, we can consider direct implicit block method [2], Chebyshev finite difference method [3], sinc collocation method [4, 5], compact finite difference method [6], non-standard finite difference method [7, 8] and rational finite difference method [9, 10]. Also, Ramos [11] presented a non-standard explicit algorithm for initial-value problems.

In this paper a new class of novel non-classical difference methods is proposed for the solution of problem (1)–(2). Our methods are based on the idea behind in [10, 11]. Two point boundary value problems (1)–(2) covers many interesting problems. Three of these important problems, which we consider in this paper, are as follows:

1.1 TROESCH'S PROBLEM

Troesch's problem is defined by

$$\begin{cases} y'' - \mu \sinh(\mu y(x)) = 0, & 0 \le x \le 1, \\ y(0) = 0, & y(1) = 1, \end{cases} \tag{3}$$

where μ is a positive constant. This problem arises in an investigation of the confinement of a plasma column under radiation pressure [12]. Also, this problem comes from the theory of gas porous electrodes [13]. Moreover, as pointed out in [14], Troesch's problems may be used to model some chemical reaction-diffusion and heat transfer processes.

The known closed-form solution of this problem in terms of the Jacobi elliptic function is (see [15])

$$y(x) = \frac{2}{\mu} \sinh^{-1}\left\{\frac{y'(0)}{2}\, \mathrm{sc}\left(\mu x \middle| 1 - \frac{1}{4} y'(0)^2\right)\right\}.$$

Here $y'(0) = 2\sqrt{1-m}$, and the constant m satisfies the transcendental equation

$$\frac{\sinh\left(\frac{\mu}{2}\right)}{\sqrt{1-m}} = \mathrm{sc}(\mu|m),$$

where, $\mathrm{sc}(\mu|m)$ is the Jacobi elliptic function. As is said in [16], this problem is inherently unstable and difficult, especially when the sensitivity parameter μ is large. Therefore, Troesch's problem has become a widely used test problem, and has been studied extensively. In the last decade, variational spline method [14], discontinuous Galerkin finite element method [17], variational iteration method [18], shooting method [19], B-spline collocation method [20], Christov collocation method [21], sinc-Galerkin method [22], nonstandard finite difference method [7], finite difference method [23] and homotopy analysis method [24] are used to solve this problem.

1.2 BRATU'S PROBLEM

The classical Bratu's problem is given as:

$$\begin{cases} y'' + \lambda \exp(y) = 0, & 0 \le x \le 1, \\ y(0) = y(1) = 0, \end{cases} \tag{4}$$

where λ is a constant. For $\lambda > 0$, the analytical solution to this problem reads [24, 25, 26, 27],

$$y(x) = -2 \ln \left[\frac{\cosh\left(\left(x - \frac{1}{2}\right)\theta/2\right)}{\cosh(\theta/4)} \right], \tag{5}$$

where θ satisfies $\theta = \sqrt{2\lambda} \cosh(\theta/4)$. It is well known that, this problem has zero, one, or two solutions when $\lambda > \lambda c$, $\lambda = \lambda c$ and $\lambda < \lambda c$, respectively. Here λc, called the critical value, is given by $\lambda c = 3.513830719$ [24, 25].

The Bratu model appears in a large variety of applications such as the model of thermal reaction process, questions in geometry and relativity about the Chandrasekhar model, radiative heat transfer, nanotechnology and the fuel ignition model of the thermal combustion theory (for example, we refer the reader to see [24, 25, 26, 27, 28, 29, 30], and the references therein). Various numerical methods such as homotopy analysis method [24], Adomian decomposition method [25, 28], sinc-Galerkin method [26], B-spline method [27], pseudospectral method [29] and finite difference method [29] have been applied to this problem. Also, recently, Temimi and Ben-Romdhane [30] proposed an iterative finite difference method to solve the Bratu's problem.

1.3 SINGULARLY PERTURBED PROBLEM

We consider a class of singularly perturbed boundary value problems given in [6, 31, 32] as

$$\begin{cases} -\epsilon y''(x) + p(x)y(x) = q(x), & 0 \le x \le 1, p(x) > 0, \\ y(0) = \alpha, \quad y(1) = \beta, \end{cases} \tag{6}$$

where α, β are given constants and $\epsilon \in (0, \epsilon_0), \epsilon_0 \ll 1$, is a small perturbation parameter. Further, $p(x)$ and $q(x)$ are assumed to be sufficiently continuously differentiable functions.

This type of problem occurs in many fields of science and engineering (see [6, 31, 32]). As pointed out in [32], usual numerical treatment of singular-perturbation problems gives major computational difficulties. This problem, has been studied by several researchers. Gelu et al. [6] used sixth-order compact finite difference method and Rashidinia et al. [31] employed quantic spline method. Khan et al. [32] solved this problem by sixth-order method based on sextic splines. Also, we refer the interested readers to [33, 34, 35, 36, 37].
The organization of the rest of this paper is as follows. In Section 2, the methods are described and also local truncation errors are discussed. In section 3, the numerical results of applying the methods of this paper on three test problems are presented. Finally a conclusion is drawn in Section 4.

2. THE PROPOSED METHODS

To approximate the solution of problem (1)–(2), first of all, the domain $[a,b]$ is divided into N equal subintervals of fixed mesh length $h = (b-a)/N$. The grid points are given by $x_i = a + ih, i = 0,\dots,N$, in which N is a positive integer. For convenience let $y^{(k)}(x_i) = y_i^{(k)}$, and $f^{(k)}\big(x_i, y(x_i)\big) = f_i^{(k)}, k = 0,1,2,\cdots$. Now, following the ideas in [11, 10], we suggest the following difference equation

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{\frac{h^2}{1+g(h)}} = f_i, \tag{7}$$

equivalently,

$$(y_{i+1} - 2y_i + y_{i-1})\big(1 + g(h)\big) = h^2 f_i, \tag{8}$$

where $g(h) \neq -1$ is a sufficiently differentiable unknown function that has to be determined. Expanding $g(h)$ in Taylor's expansion about $h = 0$ and also expanding y_{i+1} and y_{i-1} on the left side of Eq. (8) in the neighborhood of x_i by Taylor's expansion, we obtain

$$\left(h^2 y_i'' + \frac{h^4}{12} y_i^{(4)} + \frac{h^6}{360} y_i^{(6)} + \cdots\right)\left(1 + g(0) + hg'(0) + \frac{h^2}{2} g''(0) + \cdots\right) = h^2 f_i. \tag{9}$$

Now, we rewrite Eq. (9) as follows

$$\begin{aligned}
h^2\big[y_i''\big(1+g(0)\big)-f_i\big] &+ h^3[y_i''g'(0)] + h^4\left[\frac{y_i''\big(g''(0)\big)}{2}+\frac{y_i^{(4)}}{12}\big(1+g(0)\big)\right]\\
&+ h^5\left[\frac{y_i''g^{(3)}(0)}{6}+\frac{y_i^{(4)}g'(0)}{12}\right]\\
&+ h^6\left[\frac{y_i''g^{(4)}(0)}{24}+\frac{y_i^{(4)}g''(0)}{24}+\frac{y_i^{(6)}\big(1+g(0)\big)}{360}\right]+O(h^7)\\
&= 0.
\end{aligned} \tag{10}$$

In order to obtain a fourth-order scheme, the coefficients of h^2, h^3 and h^4 in Eq.(10) must be zero. So, we have

$$g(0)=0, \qquad g'(0)=0, \qquad g''(0)=-\frac{1}{6}\frac{y_i^{(4)}}{y_i''}. \tag{11}$$

By substituting the above values in the Taylor series of $g(h)$ we obtain

$$g(h)=-\frac{h^2}{12}\frac{y_i^{(4)}}{y_i''}+O(h^3). \tag{12}$$

From Eqs.(8) and (12) we get

$$(y_{i+1}-2y_i+y_{i-1})\left(1-\frac{h^2}{12}\frac{y_i^{(4)}}{y_i''}\right)-h^2f_i=0. \tag{13}$$

Therefore, using Eq. (13) and having in mind the problem (1)−(2), we obtain the numerical method given by

$$\textit{Scheme 1:}\begin{cases}(y_{i+1}-2y_i+y_{i-1})\left(1-\frac{h^2}{12}\frac{f_i^{(2)}}{f_i}\right)=h^2f_i, \quad i=1,2,\cdots,N-1,\\ y_0=\alpha,\ y_N=\beta.\end{cases} \tag{14}$$

Similarly, in order to obtain a sixth-order scheme, the coefficients of h^2, h^3, h^4, h^5 and h^6 in Eq.(10) must be zero. So, we obtain

$$\begin{aligned}
&g(0)=g'(0)=g^{(3)}(0)=0,\ g''(0)=-\frac{1}{6}\frac{y_i^{(4)}}{y_i''},\\
&g^{(4)}(0) = -\frac{y_i^{(4)}g''(0)}{y_i''}+y_i^{(6)}\frac{1+g(0)}{15y_i''}.
\end{aligned} \tag{15}$$

Therefore,

$$g(h) = -\frac{h^2}{12}\frac{y_i^{(4)}}{y_i''} + \frac{h^4}{y_i''}\left(\frac{1}{144}\frac{\left(y_i^{(4)}\right)^2}{y_i''} - \frac{y_i^{(6)}}{360}\right) + O(h^5). \tag{16}$$

Employing Eqs. (1), (2), (16) and (8), we obtain the numerical method given by

$$\textit{Scheme 2}: \begin{cases} (y_{i+1} - 2y_i + y_{i-1})\left(1 - \frac{h^2}{12}\frac{f_i^{(2)}}{f_i} + \frac{h^4}{f_i}\left(\frac{\left(f_i^{(2)}\right)^2}{144 f_i} - \frac{f_i^{(4)}}{360}\right)\right) = h^2 f_i, \\ i = 1,2,\cdots,N-1, \\ y_0 = \alpha,\ y_N = \beta\,. \end{cases} \tag{17}$$

2.1 LOCAL TRUNCATION ERROR

It follows from the construction of the methods in Eqs. (14) and (17) that the new *Scheme 1* and *Scheme 2* are at least of fourth-order and sixth-order respectively. In fact, for *Scheme 1*, let us define

$$LTE_i^1 = (y(x_i + h) - 2y(x_i) + y(x_i - h))\left(1 - \frac{h^2}{12}\frac{f^{(2)}(x_i, y(x_i))}{f(x_i, y(x_i))}\right) - h^2 f(x_i, y(x_i)). \tag{18}$$

After expanding each term on the right side of Eq. (18) in Taylor series about x_i and collecting terms in h we get

$$LTE_i^1 = \left(-\frac{1}{144}\frac{\left(y^{(4)}(x_i)\right)^2}{y''(x_i)} + \frac{1}{360}y^{(6)}(x_i)\right)h^6 + O(h^8). \tag{19}$$

Similarly, for *Scheme 2*, we have

$$LTE_i^2 = \left(\frac{1}{1728}\frac{\left(y^{(4)}(x_i)\right)^3}{\left(y''(x_i)\right)^2} - \frac{1}{2160}\frac{y^{(4)}(x_i)y^{(6)}(x_i)}{y''(x_i)} + \frac{1}{20160}y^{(8)}(x_i)\right)h^8 + O(h^{10}). \tag{20}$$

3. NUMERICAL RESULTS

In this section, to validate the application of the presented methods to problem (1)–(2), we consider three test problems. We have computed the numerical results by Maple programming.

Example 1. (*Troesch's problem*) In this example we will consider Troesch's problem given in Eq. (3) for different values of the parameter μ. We solved this problem, by applying the techniques described in Section 2. Taking $\mu = 0.5$ and $\mu = 1$, in Tables 1 and 2 we compare our results with the exact solutions given in [7]. Also, in Table 3 the numerical solution obtained by *Scheme 1* and *Scheme 2* for $\mu = 5$ is compared with the numerical approximation of the exact solutions given by a Fortran code [20] and the numerical solution obtained by B-spline collocation method [20]. From Tables 1–3 we see that *Scheme1* and *Scheme 2* yields a reasonable numerical solution for $\mu = 0.5, 1$ and 5. As said in [20, 23], the stiffness ratio near $x = 1$ increases as μ increases. For this reason, most common numerical methods fail to provide enough accurate solutions for large values of μ. In Table 4 the numerical solution obtained by the *Scheme 2* with $N = 300$, for $\mu = 10, 30$, is compared with the results obtained in [20] by the adaptive collocation method over a non-uniform mesh using $N = 330$ and those obtained in [23] by finite difference method (FDM) for mesh size $N = 2000$. It can be seen from Table 4 that the results obtained using Scheme 2 have a good agreement with the results obtained in [20, 23].

Table 1: Results for Troesch's problem ($\mu = 0.5$).

x	Exact	*Scheme1*		*Scheme2*	
		$N = 10$	$N = 20$	$N = 10$	$N = 20$
0.1	0.0959443493	5.0(-10)	1.0(-10)	8.0(-10)	1.0(-10)
0.2	0.1921287477	1.0(-9)	1.0(-10)	1.4(-9)	1.0(-10)
0.3	0.2887944009	1.3(-9)	1.0(-10)	2.0(-9)	0
0.4	0.3861848464	1.7(-9)	1.0(-10)	1.0(-10)	0
0.5	0.4845471647	1.8(-9)	1.0(-10)	2.7(-9)	0
0.6	0.5841332484	1.9(-9)	1.0(-10)	2.8(-9)	0
0.7	0.6852011483	1.8(-9)	1.0(-10)	2.7(-9)	1.0(-10)
0.8	0.7880165227	1.5(-9)	1.0(-10)	2.3(-9)	1.0(-10)
0.9	0.8928542161	9.0(-9)	0	1.3(-9)	0

Example 2. (*Bratu's problem*) As the second example, we consider Bratu's problem given in Eq. (4) for different values of the parameter λ. Taking $\lambda = 1, 2$, Tables 5 and 6, show the numerical solution obtained by our methods with $N = 200$ compared to the exact solution given by Eq. (5), as well as to the values computed by iterative finite difference (IFD) method with $N = 1000$ given in [30] and B-spline method given in [27]. Moreover, for the critical value $\lambda = 3.51$, in Table 7 the numerical solution obtained by the present methods with $N = 300$, is compared with the B-spline method [27] and IFD method [30]. As pointed by [30], many existing numerical methods for Bratu's problem fail to compute the solution for $\lambda = 3.51$. From Tables 5–7, we see that the present methods are in excellent agreement with the exact values and the IFD method. Also, the present methods are clearly reliable if compared with the B-spline method.

Table 2: Results for Troesch's problem ($\mu = 1$).

x	Exact	*Scheme 1*		*Scheme 2*	
		$N = 10$	$N = 20$	$N = 10$	$N = 20$
0.1	0.0846612565	2.6(-8)	1.7(-9)	4.3(-8)	2.7(-9)
0.2	0.1701713582	5.2(-8)	3.3(-9)	8.4(-8)	5.4(-9)
0.3	0.2573939080	7.6(-8)	4.7(-9)	1.2(-7)	7.8(-9)
0.4	0.3472228551	9.7(-8)	6.1(-9)	1.5(-7)	1.0(-8)
0.5	0.4405998351	1.1(-7)	7.0(-9)	1.8(-7)	1.1(-8)
0.6	0.5385343980	1.2(-7)	7.6(-9)	2.0(-7)	1.2(-8)
0.7	0.6421286091	1.2(-7)	7.5(-9)	2.0(-7)	1.2(-8)
0.8	0.7526080939	1.0(-7)	6.5(-9)	1.7(-7)	1.1(-8)
0.9	0.8713625196	6.9(-8)	4.1(-9)	1.1(-7)	7.3(-9)

Example 3. Consider the following singularly perturbed problem [6, 31]:

$$\begin{cases} -\epsilon y'' + y = x, \quad 0 \le x \le 1, \\ y(0) = 1, \quad y(1) = 1 + \exp\left(\frac{1}{\sqrt{\epsilon}}\right). \end{cases} \tag{21}$$

The exact solution of this problem is

$$y(x) = x + \exp\left(-\frac{x}{\sqrt{\epsilon}}\right). \tag{22}$$

This problem is solved in [6] by sixth-order compact finite difference method. Also, in [31] the authors used quintic spline method to solve this problem. For the purpose of comparison in Table 8, we compare maximum absolute errors of our methods, for different values of ϵ and N, together with the maximum absolute errors given in [6, 31].

Furthermore, we have calculated the computational orders of our methods (denoted by C-order) with the following formula:

$$\frac{\log(E_N) - \log(E_{2N})}{\log(2)},$$

where E_N and E_{2N} are maximum absolute errors obtained using N and $2N$ mesh intervals, respectively. The results are summarized in Tables 9 and 10. From Tables 9 and 10, we see that the computational and theoretical orders of Scheme 1 and Scheme 2 are very close to each other, i.e the order of *Scheme 1* and *Scheme 2* are $O(h^4)$ and $O(h^6)$, respectively.

4. CONCLUSION

In this paper, a new family of schemes for numerically solving two point boundary value problems is presented. We showed that, the order of *Scheme 1* and *Scheme 2* are $O(h^4)$ and $O(h^6)$, respectively. These schemes are used for solving Troesch's problem, Bratu's problem and certain singularly perturbed problem. According to the numerical results, *Scheme 1* and *Scheme 2* can handle these kind of problems effectively and the comparison show that the proposed methods are in good agreement with the existing results in the literature. Also numerical results confirm the theoretical results of the proposed techniques.

Table 3: Comparison of numerical solutions for Troesch's problem ($\mu = 5$).

x	Fortran code [20]	*Scheme 1* N = 20	*Scheme 2* N = 20	B-spline [20]
0.2	0.01075342	0.01071950	0.01070406	0.01002027
0.4	0.03320051	0.03309592	0.03304801	0.03099793
0.6	0.25821664	0.25735421	0.25695699	0.24170496
0.8	0.45506034	0.45335039	0.45258050	0.42461830

Table 4: Comparison of numerical solutions for Troesch's problem ($\mu = 10, 30$).

	$\mu = 10$			$\mu = 30$	
	Scheme 2	B-spline[20]	FDM	*Scheme 2*	FDM[23]
x	N = 300	N = 330	N = 2000	N = 300	N = 2000
0	0	0	0	0	0
0.1	4.204824(−5)	4.207335(−5)	4.211194(−5)	3.614375(−13)	2.500056(−13)
0.2	1.297676(−4)	1.298517(−4)	1.299642(−4)	7.277661(−12)	5.033929(−12)
0.3	3.584358(−4)	3.586905(−4)	3.589786(−4)	1.461766(−10)	1.011094(−10)
0.4	9.764246(−4)	9.771828(−4)	9.779034(−4)	2.936036(−9)	2.030831(−9)
0.5	2.655001(−3)	2.657239(−3)	2.659022(−3)	5.897186(−8)	4.079021(−8)
0.6	7.218002(−3)	7.224571(−3)	7.228934(−3)	1.184481(−6)	8.192908(−7)
0.7	1.963429(−2)	1.965351(−2)	1.966406(−2)	2.379094(−5)	1.645584(−5)
0.8	5.364813(−2)	5.370517(−2)	5.373034(−2)	4.778560(−4)	3.305241(−4)
0.9	1.518614(−1)	1.520568(−1)	1.521140(−1)	9.614584(−3)	6.644214(−3)
0.95	2.757046(−1)	2.761735(−1)		4.460814(−2)	3.026175(−2)
0.97	3.713175(−1)	3.721473(−1)		8.991531(−2)	5.753674(−2)
0.98	4.468330(−1)	4.481030(−1)		1.441330(−1)	8.223035(−2)
0.99	5.714501(−1)	5.739404(−1)		5.218877(−1)	1.269861(−1)
1	1	1	1	1	1

Table 5: Comparison of numerical solutions for Bratu's problem ($\lambda = 1$).

x	Exact	*Scheme 1*	*Scheme 2*	B-spline[27]	IDF[30]
0.1	0.049846791245	0.049846791245	0.049846791245	0.0498438103	0.049846791445
0.2	0.089189934629	0.089189934628	0.089189934629	0.0891844690	0.089189934988
0.3	0.117609095768	0.117609095767	0.117609095768	0.1176017599	0.117609096243
0.4	0.134790253884	0.134790253883	0.134790253884	0.1347817559	0.134790254431
0.5	0.140539214400	0.140539214399	0.140539214400	0.1405303221	0.140539214971
0.6	0.134790253884	0.134790253883	0.134790253884	0.1347817559	0.134790254430
0.7	0.117609095768	0.117609095767	0.117609095768	0.1176017599	0.117609096243
0.8	0.089189934629	0.089189934628	0.089189934629	0.0891844690	0.089189934988
0.9	0.049846791245	0.049846791245	0.049846791245	0.0498438103	0.049846791444

Table 6: Comparison of numerical solutions for Bratu's problem ($\lambda = 2$).

x	Exact	*Scheme 1*	*Scheme 2*	B-spline[27]	IDF[30]
0.1	0.114410743268	0.114410743264	0.114410743265	0.1143935651	0.114410743957
0.2	0.206419116488	0.206419116481	0.206419116483	0.2063865190	0.206419117764
0.3	0.273879311826	0.273879311817	0.273879311820	0.2738344125	0.273879313548
0.4	0.315089364226	0.315089364215	0.315089364220	0.3150365062	0.315089366227
0.5	0.328952421341	0.328952421330	0.328952421335	0.3288968072	0.328952423437
0.6	0.315089364226	0.315089364215	0.315089364220	0.3150365062	0.315089366228
0.7	0.273879311826	0.273879311817	0.273879311820	0.2738344125	0.273879313550
0.8	0.206419116488	0.206419116481	0.206419116483	0.2063865190	0.206419117767
0.9	0.114410743268	0.114410743264	0.114410743265	0.1143935651	0.114410743961

Table 7: Comparison of numerical solutions for Bratu's problem ($\lambda = 3.51$).

x	Exact	*Scheme 1*	*Scheme 2*	B-spline[27]	IDF[30]
0.1	0.364335803565	0.364335803086	0.364335802967	0.357388461	0.364335803565
0.2	0.677869705682	0.677869704751	0.677869704528	0.664283874	0.677869705683
0.3	0.922214197098	0.922214195783	0.922214195480	0.902930838	0.922214197097
0.4	1.078634240752	1.078634239178	1.078634238825	1.055419782	1.078634240752
0.5	1.132617978282	1.132617976616	1.132617976246	1.107989815	1.132617978283
0.6	1.078634240752	1.078634239178	1.078634238825	1.055419782	1.078634240752
0.7	0.922214197097	0.922214195783	0.922214195480	0.902930838	0.922214197097
0.8	0.677869705682	0.677869704751	0.677869704528	0.664283874	0.677869705683
0.9	0.364335803565	0.364335803086	0.364335802967	0.357388461	0.364335803565

Table 8: Comparison of maximum absolute errors for Example 3.

ϵ	N = 16	N = 32	N = 64
Scheme 1			
1/16	2.96(−6)	1.85(−7)	1.15(−8)
1/32	1.19(−5)	7.45(−7)	4.67(−8)
1/64	4.74(−5)	2.98(−6)	1.87(−7)
1/128	1.78(−4)	1.19(−5)	7.46(−7)
Scheme 2			
1/16	7.34(−9)	1.14(−10)	1.79(−12)
1/32	5.90(−8)	9.25(−10)	1.45(−11)
1/64	4.71(−7)	7.41(−9)	1.16(−10)
1/128	3.54(−6)	5.90(−8)	9.25(−10)
Method of [6]			
1/16	8.03(−9)	1.26(−10)	1.97(−12)
1/32	6.41(−8)	1.01(−9)	1.59(−11)
1/64	5.06(−7)	8.10(−9)	1.27(−10)
1/128	3.72(−6)	6.42(−8)	1.01(−9)
Method of [31]			
1/16	2.96(−6)	1.85(−7)	1.15(−8)
1/32	1.18(−5)	7.54(−7)	4.67(−8)
1/64	4.74(−5)	2.96(−6)	1.86(−7)
1/128	1.78(−4)	1.18(−5)	7.46(−7)

Table 9: Errors and computational orders obtained by *Scheme 1*, for Example 3.

	$\epsilon = 1/16$		$\epsilon = 1/32$		$\epsilon = 1/64$	
N	E_N	C-order	E_N	C-order	E_N	C-order
16	2.96(−6)	--	1.19(−5)	--	4.74(−5)	--
32	1.85(−7)	3.9999	7.45(−7)	3.9975	2.98(−6)	3.9915
64	1.15(−8)	4.0078	4.67(−8)	3.9957	1.87(−7)	3.9942
128	7.26(−10)	3.9855	2.92(−9)	3.9993	1.16(−8)	4.0108

Table 10: Errors and computational orders obtained by *Scheme 2*, for Example 3.

	$\epsilon = 1/16$		$\epsilon = 1/32$		$\epsilon = 1/64$	
N	E_N	C-order	E_N	C-order	E_N	C-order
16	7.34(−9)	--	5.90(−8)	--	4.71(−7)	--
32	1.14(−10)	6.0086	9.25(−10)	5.9951	7.41(−9)	5.9901
64	1.79(−12)	5.9929	1.45(−11)	5.9953	1.16(−10)	5.9972
128	2.80(−14)	5.9983	2.26(−13)	6.0035	1.81(−12)	6.0019

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On Reciprocal Complementary Wiener Index of a Graph

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ABSTRACT

The eccentricity of a vertex v of G is the largest distance between v and any other vertex in G. The reciprocal complementary Wiener (RCW) index of G is defined as

$$RCW(G) = \sum_{1 \le i < j \le n} \frac{1}{1+D-d(v_i,v_j)},$$

where D is the diameter of G and $d(v_i,v_j)$ is the distance between the vertices v_i and v_j. In this paper, we have obtained bounds for the RCW index in terms of eccentricities and given an algorithm to compute the RCW index.

1 INTRODUCTION

Graph theory has provided chemist with a variety of useful tools, such as Topological Index. Molecules and molecular compounds are often modeled by molecular graph. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to the chemical bonds.

Throughout this paper we consider only simple, connected graphs without loops and multiple edges [1]. Let G be such graph with n vertices, m edges and vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$. The *degree* of $v_i \in V(G)$, denoted by $deg(v_i)$, is the number of vertices adjacent to v_i. The sum of the degrees of the vertices of G is $2m$. The *distance* between the vertices

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v_i and v_j of $V(G)$, denoted by $d(v_i, v_j)$, is the length of the shortest path joining them. The *eccentricity* of a vertex $v \in V(G)$, denoted by $e(v)$, is the largest distance between v and any other vertex of the graph G. The *radius* $r = r(G)$ of G is the minimum eccentricity of the vertices and the *diameter* $D = D(G)$ of G is the maximum eccentricity. A vertex v is called *central vertex* of G, if $e(v) = r(G)$. A graph is called *self-centered* if every vertex is a central vertex. Thus in a self-centered graph $r(G) = D(G)$. A vertex u is said to be an *eccentric vertex* of a vertex v if $d(u, v) = e(v)$. An *eccentric path* $P(v)$ of a vertex v is a path of length $e(v)$ joining v and its eccentric vertex. There may exist more than one eccentric path for a given vertex.

A topological index is a graph invariant applicable in chemistry. The Wiener index is the first topological index introduced by Harold Wiener in 1947 [11]. There are many topological indices which are frequently made their appearance in both chemical and mathematical literature.

Wiener index $W(G)$ of a graph G is defined as [11],

$$W(G) = \sum_{1 \le i < j \le n} d(v_i, v_j). \tag{1}$$

The *reciprocal complementary Wiener* (*RCW*) index of a graph G is defined as [3, 4]

$$RCW(G) = \sum_{1 \le i < j \le n} \frac{1}{1 + D - d(v_i, v_j)}, \tag{2}$$

where D is the diameter of G.

The reciprocal complementary distance number of vertex v_i of G, denoted by $RCDN(v_i \mid G)$ is defined as,

$$RCDN(v_i \mid G) = \sum_{j=1}^{n} \frac{1}{1 + D - d(v_i, v_j)}.$$

Therefore, $RCW(G) = \frac{1}{2} \sum_{i=1}^{n} RCDN(v_i \mid G)$.

The chemical applications of *RCW* index are reported in the literature [3−5, 10] and one can refer the mathematical properties of *RCW* index in [2, 6, 8, 12−14]. *RCW* index has been successfully applied in the structure property modeling of the molar heat capacity, standard Gibbs energy of formation and vaporization enthalpy of 134 alkanes $C_6 - C_{10}$ [3]. In [2] Cai and Zhou determined the trees with the smallest, the second smallest and the third smallest *RCW* indices, and the unicyclic and bicyclic graphs with the smallest and the second smallest *RCW* indices. In [13] Zhou et al. obtained some properties, especially various upper and lower bounds and Nordhaus-Gaddum-type results of *RCW* indices. Qi and Zhou [6] characterized the trees with fixed number of vertices and matching number with the smallest *RCW* index. Ramane et al. [7, 9] obtained bounds for the Wiener number and also for Harary index in terms of eccentricities. The present work contains bounds on the RCW index in terms of eccentricities and moreover, we have given a simple algorithm to compute RCW index for any simple graph.

2. MAIN RESULTS

Theorem 1. Let G be a simple, connected graph with n vertices, m edges, diameter D and $e_i = e(v_i)$, for $i = 1,2,...,n$. Then,

$$RCW(G) \geq \frac{1}{2}\left[\frac{n(n-1)-\sum_{i=1}^{n} e_i}{D-1} - \frac{2m-n}{D(D-1)} + \sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{D-(j-1)}\right]. \quad (3)$$

Equality holds if and only if for every vertex v_i of G, if $P(v_i)$ is one of the eccentric path of v_i, then for every $v_j \in V(G)$ which is not on $P(v_i)$, $d(v_i, v_j) \leq 2$.

Proof. Let $P(v_i)$ be one of the eccentric path of $v_i \in V(G)$. Let

$A_1(v_i) = \{v_j \mid v_j$ is on eccentric path $P(v_i)$ of $v_i\}$,

$A_2(v_i) = \{v_j \mid v_j$ is adjacent to v_i and which is not on the eccentric path $P(v_i)$ of $v_i\}$,

$A_3(v_i) = \{v_j \mid v_j$ is not adjacent to v_i and not on the eccentric path $P(v_i)$ of $v_i\}$.

It is clear that $A_1(v_i) \cup A_2(v_i) \cup A_3(v_i) = V(G)$ and $|A_1(v_i)| = e_i + 1$, $|A_2(v_i)| = deg(v_i) - 1$, $|A_3(v_i)| = n - e_i - deg(v_i)$. Now

$$\sum_{v_j \in A_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \sum_{j=1}^{e_i}\frac{1}{D-(j-1)}, \quad \sum_{v_j \in A_2(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \frac{deg(v_i)-1}{D},$$

$$\sum_{v_j \in A_3(v_i)} \frac{1}{1+D-d(v_i,v_j)} \geq \frac{n-e_i-deg(v_i)}{D-1} .$$

Therefore,

$$\begin{aligned} RCDN(v_i \mid G) &= \sum_{j=1}^{n}\frac{1}{1+D-d(v_i,v_j)} \\ &= \sum_{v_j \in A_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \sum_{v_j \in A_2(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \\ &\quad \sum_{v_j \in A_3(v_i)} \frac{1}{1+D-d(v_i,v_j)} \\ &\geq \frac{D(n-e_i-1)-deg(v_i)+1}{D(D-1)} + \sum_{j=1}^{e_i}\frac{1}{D-(j-1)} . \end{aligned}$$

Therefore,

$$
\begin{aligned}
RCW(G) &= \frac{1}{2}\sum_{i=1}^{n} RCDN(v_i \mid G) \\
&\geq \frac{1}{2}\sum_{i=1}^{n}\left[\frac{D(n-e_i-1)-deg(v_i)+1}{D(D-1)}+\sum_{j=1}^{e_i}\frac{1}{D-(j-1)}\right] \\
&= \frac{1}{2}\left[\frac{n(n-1)-\sum_{i=1}^{n} e_i}{D-1}-\frac{2m-n}{D(D-1)}+\sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{D-(j-1)}\right].
\end{aligned}
$$

For equality, Let $d(v_i,v_j) = 2$, where $v_j \in A_3(v_i)$. Therefore

$$
\sum_{v_j \in A_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \sum_{j=1}^{e_i}\frac{1}{D-(j-1)}, \qquad \sum_{v_j \in A_2(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \frac{\deg(v_i)-1}{D},
$$

$$
\sum_{v_j \in A_3(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \frac{n-e_i-deg(v_i)}{D-1}.
$$

Thus

$$
\begin{aligned}
RCDN(v_i \mid G) &= \sum_{j=1}^{n}\frac{1}{1+D-d(v_i,v_j)} \\
&= \sum_{v_j \in A_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \sum_{v_j \in A_2(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \\
&\quad \sum_{v_j \in A_3(v_i)} \frac{1}{1+D-d(v_i,v_j)} \\
&= \frac{D(n-e_i-1)-deg(v_i)+1}{D(D-1)}+\sum_{j=1}^{e_i}\frac{1}{D-(j-1)}.
\end{aligned}
$$

Hence

$$
\begin{aligned}
RCW(G) &= \frac{1}{2}\sum_{i=1}^{n} RCDN(v_i \mid G) \\
&= \frac{1}{2}\left[\frac{n(n-1)-\sum_{i=1}^{n} e_i}{D-1}-\frac{2m-n}{D(D-1)}+\sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{D-(j-1)}\right].
\end{aligned}
$$

Conversely, suppose G is not such as explained in the equality part of this theorem. Then there exist at least one vertex $v_j \in A_3(v_i)$ such that $d(v_i, v_j) \geq 3$. Let $A_3(v_i)$ be partitioned into two sets $A_{31}(v_i)$ and $A_{32}(v_i)$, where

$A_{31}(v_i) = \{v_j \mid v_j$ is not adjacent to v_i, not on the eccentric path $P(v_i)$ of v_i and $d(v_i, v_j) = 2\}$,

$A_{32}(v_i) = \{v_j \mid v_j$ is not adjacent to v_i, not on the eccentric path $P(v_i)$ of v_i and $d(v_i, v_j) \geq 3\}$. Let $|A_{32}(v_i)| = l \geq 1$. So, $|A_{31}(v_i)| = n - e_i - deg(v_i) - l$. Therefore

$$\sum_{v_j \in A_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \sum_{j=1}^{e_i} \frac{1}{D-(j-1)}, \quad \sum_{v_j \in A_2(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \frac{\deg(v_i)-1}{D},$$

$$\sum_{v_j \in A_{31}(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \frac{n-e_i-deg(v_i)-l}{D-1}, \quad \sum_{v_j \in A_{32}(v_i)} \frac{1}{1+D-d(v_i,v_j)} \geq \frac{l}{D-2}.$$

Therefore,

$$\begin{aligned}
RCDN(v_i \mid G) &= \sum_{j=1}^{n} \frac{1}{1+D-d(v_i,v_j)} \\
&= \sum_{v_j \in A_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \sum_{v_j \in A_2(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \\
&\quad \sum_{v_j \in A_{31}(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \sum_{v_j \in A_{32}(v_i)} \frac{1}{1+D-d(v_i,v_j)} \\
&= \frac{D(n-e_i-1)-deg(v_i)+1}{D(D-1)} + \sum_{j=1}^{e_i} \frac{1}{D-(j-1)} \\
&\quad + \frac{l}{(D-2)(D-1)}
\end{aligned}$$

and so

$$\begin{aligned}
RCW(G) &= \frac{1}{2} \sum_{i=1}^{n} RCDN(v_i \mid G) \\
&\geq \frac{1}{2} \sum_{i=1}^{n} \left[\begin{aligned} &\frac{D(n-e_i-1)-deg(v_i)+1}{D(D-1)} + \sum_{j=1}^{e_i} \frac{1}{D-(j-1)} \\ &+ \frac{l}{(D-2)(D-1)} \end{aligned} \right] \\
&= \frac{1}{2} \left[\begin{aligned} &\frac{n(n-1)-\sum_{i=1}^{n} e_i}{D-1} - \frac{2m-n}{D(D-1)} + \sum_{i=1}^{n} \sum_{j=1}^{e_i} \frac{1}{D-(j-1)} \\ &+ \frac{nl}{(D-2)(D-1)} \end{aligned} \right].
\end{aligned}$$

This is a contradiction to the equality as $l \geq 1$. This completes the proof. □

Corollary 2. Let G be a self-centered graph with n vertices, m edges and radius $r = r(G)$. Then

$$RCW(G) \geq \frac{1}{2}\left[\frac{nr(n-1-r)-2m+n}{r(r-1)} + n\sum_{j=1}^{r}\frac{1}{r-(j-1)}\right]. \tag{4}$$

Equality holds if and only if for every vertex v_i of a self-centered graph G, if $P(v_i)$ is one of the eccentric path of v_i then for every $v_j \in V(G)$ which is not on the eccentric path $P(v_i)$, $d(v_i, v_j) \leq 2$.

Proof. Since G is a self-centered graph, the radius $r = e_i = e(v_i) = D$ for $i = 1, 2, \ldots, n$. Therefore by Eq. (3)

$$RCW(G) \geq \frac{1}{2}\left[\frac{n(n-1-r)}{r-1} - \frac{2m-n}{r(r-1)} + \sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{r-(j-1)}\right]$$
$$= \frac{1}{2}\left[\frac{nr(n-1-r)-2m+n}{r(r-1)} + n\sum_{j=1}^{r}\frac{1}{r-(j-1)}\right].$$

Equality part can be proved in analogous to the proof of equality part of Theorem 1. □

Theorem 3. Let G be a connected graph with n vertices and $e_i = e(v_i)$, $i = 1, 2, \ldots, n$. Then

$$RCW(G) \geq \frac{1}{2}\left[\frac{n(n-1)-\sum_{i=1}^{n} e_i}{D} + \sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{D-(j-1)}\right]. \tag{5}$$

Equality holds if and only if for every vertex v_i of G, if $P(v_i)$ is one of the eccentric path of v_i, then for every $v_j \in V(G)$ which is not on $P(v_i)$, $d(v_i, v_j) = 1$.

Proof. Let $P(v_i)$ be one of the eccentric path of $v_i \in V(G)$, $B_1(v_i) = \{v_j \mid v_j$ is on eccentric path $P(v_i)$ of $v_i\}$ and $B_2(v_i) = \{v_j \mid v_j$ is not on the eccentric path $P(v_i)$ of $v_i\}$. It is easy to check that $B_1(v_i) \cup B_2(v_i) = V(G)$, $|B_1(v_i)| = e_i + 1$ and $|B_2(v_i)| = n - e_i - 1$. Now

$$\sum_{v_j \in B_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \sum_{j=1}^{e_i}\frac{1}{D-(j-1)}, \quad \sum_{v_j \in B_2(v_i)} \frac{1}{1+D-d(v_i,v_j)} \geq \frac{n-e_i-1}{D}.$$

Therefore

$$RCDN(v_i \mid G) = \sum_{j=1}^{n}\frac{1}{1+D-d(v_i,v_j)}$$
$$= \sum_{v_j \in B_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \sum_{v_j \in B_2(v_i)} \frac{1}{1+D-d(v_i,v_j)}$$
$$\geq \sum_{j=1}^{e_i}\frac{1}{D-(j-1)} + \frac{n-e_i-1}{D}.$$

Therefore

$$RCW(G) = \frac{1}{2}\sum_{i=1}^{n} RCDN(v_i \mid G)$$

$$\geq \frac{1}{2}\sum_{i=1}^{n}\left[\sum_{j=1}^{e_i}\frac{1}{D-(j-1)} + \frac{n-e_i-1}{D}\right]$$

$$= \frac{1}{2}\left[\frac{n(n-1)-\sum_{i=1}^{n} e_i}{D} + \sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{D-(j-1)}\right].$$

For equality, let $d(v_i,v_j) = 1$, where $v_j \in B_2(v_i)$. Hence

$$\sum_{v_j \in B_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \sum_{j=1}^{e_i}\frac{1}{D-(j-1)} \text{ and } \sum_{v_j \in B_2(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \frac{n-e_i-1}{D}.$$

Therefore

$$RCDN(v_i \mid G) = \sum_{j=1}^{n}\frac{1}{1+D-d(v_i,v_j)}$$

$$= \sum_{v_j \in B_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \sum_{v_j \in B_2(v_i)} \frac{1}{1+D-d(v_i,v_j)}$$

$$= \sum_{j=1}^{e_i}\frac{1}{D-(j-1)} + \frac{n-e_i-1}{D}.$$

Therefore

$$RCW(G) = \frac{1}{2}\sum_{i=1}^{n} RCDN(v_i \mid G)$$

$$= \frac{1}{2}\left[\frac{n(n-1)-\sum_{i=1}^{n} e_i}{D} + \sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{D-(j-1)}\right].$$

Conversely, suppose G is not a such graph as explained in the equality part of this theorem. Then there exist at least one vertex $v_j \in B_2(v_i)$ such that $d(v_i, v_j) \geq 2$. Let $B_2(v_i)$ be partitioned into two sets $B_{21}(v_i)$ and $B_{22}(v_i)$, where $B_{21}(v_i) = \{v_j \mid v_j$ is not on the eccentric path $P(v_i)$ of v_i and $d(v_i, v_j) = 1\}$, $B_{22}(v_i) = \{v_j \mid v_j$ is not on the eccentric path $P(v_i)$ of v_i and $d(v_i, v_j) \geq 2\}$. Let $|B_{22}(v_i)| = l \geq 1$ and $|B_{21}(v_i)| = n - e_i - 1 - l$. Therefore

$$\sum_{v_j \in B_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \sum_{j=1}^{e_i} \frac{1}{D-(j-1)}, \quad \sum_{v_j \in B_{21}(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \frac{n-e_i-1-l}{D},$$

$$\sum_{v_j \in B_{22}(v_i)} \frac{1}{1+D-d(v_i,v_j)} \geq \frac{l}{D-1}.$$

Therefore

$$RCDN(v_i \mid G) = \sum_{j=1}^{n} \frac{1}{1+D-d(v_i,v_j)}$$

$$= \sum_{v_j \in B_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \sum_{v_j \in B_{21}(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \sum_{v_j \in B_{22}(v_i)} \frac{1}{1+D-d(v_i,v_j)}$$

$$= \sum_{j=1}^{e_i} \frac{1}{D-(j-1)} + \frac{n-e_i-1-l}{D} + \frac{l}{D-1}.$$

Therefore

$$RCW(G) = \frac{1}{2}\sum_{i=1}^{n} RCDN(v_i \mid G)$$

$$\geq \frac{1}{2}\sum_{i=1}^{n}\left[\sum_{j=1}^{e_i} \frac{1}{D-(j-1)} + \frac{n-e_i-1-l}{D} + \frac{l}{D-1}\right]$$

$$= \frac{1}{2}\left[\sum_{i=1}^{n}\sum_{j=1}^{e_i} \frac{1}{D-(j-1)} + \frac{n(n-1)-\sum_{i=1}^{n} e_i}{D} + \frac{nl}{D(D-1)}\right].$$

As $l \geq 1$, it contradicts to the equality. This completes the proof. □

If G is a self-centered graph then $e_i = e(v_i) = r(G)$ for all $i = 1, 2, \ldots, n$. Substituting this in Eq. (5) we get the following corollary.

Corollary 4. Let G be a self-centered graph with n vertices and radius $r = r(G)$. Then

$$RCW(G) \geq \frac{1}{2}\left[\frac{n(n-1-r)}{r} + n\sum_{j=1}^{r} \frac{1}{r-(j-1)}\right]. \tag{6}$$

Equality holds if and only if for every vertex v_i of a self-centered graph G, if $P(v_i)$ is one of the eccentric path of v_i then for every $v_j \in V(G)$ which is not on the eccentric path $P(v_i)$, then $d(v_i, v_j) = 1$.

Theorem 5. Let G be a connected graph with n vertices, m edges and diameter D. Let e_i = e(v_i), i= 1, 2, … ,n. Then

$$RCW(G) \le \frac{1}{2}\left[n^2 - \sum_{i=1}^{n} e_i - 2m + \frac{2m-n}{D} + \sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{D-(j-1)}\right]. \tag{7}$$

Equality holds if and only if $D \le 2$.

Proof. Let $P(v_i)$ be one of the eccentric path of $v_i \in V(G)$. Let
$A_1(v_i) = \{v_j \mid v_j$ is on the eccentric path $P(v_i)$ of $v_i\}$,
$A_2(v_i) = \{v_j \mid v_j$ is adjacent to v_i and which is not on the eccentric path $P(v_i)$ of $v_i\}$,
$A_3(v_i) = \{v_j \mid v_j$ is not adjacent to v_i and not on the eccentric path $P(v_i)$ of $v_i\}$.
It is easy to check that $A_1(v_i) \cup A_2(v_i) \cup A_3(v_i) = V(G)$ and $|A_1(v_i)| = e_i + 1$, $|A_2(v_i)| = deg(v_i) - 1$ and $|A_3(v_i)| = n - e_i - deg(v_i)$. Now

$$\sum_{v_j \in A_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \sum_{j=1}^{e_i}\frac{1}{D-(j-1)}, \qquad \sum_{v_j \in A_2(v_i)} \frac{1}{1+D-d(v_i,v_j)} = \frac{deg(v_i)-1}{D},$$

$$\sum_{v_j \in A_3(v_i)} \frac{1}{1+D-d(v_i,v_j)} \le n - e_i - deg(v_i).$$

Therefore

$$\begin{aligned}
RCDN(v_i \mid G) &= \sum_{j=1}^{n}\frac{1}{1+D-d(v_i,v_j)} \\
&= \sum_{v_j \in A_1(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \sum_{v_j \in A_2(v_i)} \frac{1}{1+D-d(v_i,v_j)} + \\
&\quad \sum_{v_j \in A_3(v_i)} \frac{1}{1+D-d(v_i,v_j)} \\
&\le \sum_{j=1}^{e_i}\frac{1}{D-(j-1)} + \frac{deg(v_i)-1}{D} + (n - e_i - deg(v_i)) \\
&= \frac{D(n-e_i)+(1-D)deg(v_i)-1}{D} + \sum_{j=1}^{e_i}\frac{1}{D-(j-1)}.
\end{aligned}$$

Thus

$$\begin{aligned}
RCW(G) &= \frac{1}{2}\sum_{i=1}^{n} RCDN(v_i \mid G) \\
&\le \frac{1}{2}\sum_{i=1}^{n}\left[\frac{D(n-e_i)+(1-D)deg(v_i)-1}{D} + \sum_{j=1}^{e_i}\frac{1}{D-(j-1)}\right]
\end{aligned}$$

$$=\frac{1}{2}\left[n^2-\sum_{i=1}^{n}e_i-2m+\frac{2m-n}{D}+\sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{D-(j-1)}\right].$$

For equality, let $D \le 2$. We consider here two cases.

Case 1: If $D = 1$, then $G = K_n$, a complete graph on n vertices. Therefore, $A_3(v_i)$ is an empty set. Hence

$$RCW(G)=\frac{1}{2}\left[n^2-\sum_{i=1}^{n}e_i-n+\sum_{i=1}^{n}1\right]=\frac{n(n-1)}{2}.$$

Case 2: If $D = 2$, then for $v_j \in A_3(v_i)$, $d(v_i, v_j) = 2$. Therefore,

$$\sum_{v_j\in A_3(v_i)}\frac{1}{1+D-d(v_i,v_j)}=n-e_i-deg(v_i).$$

Hence

$$RCW(G)=\frac{1}{2}\left[n\left(n-\frac{1}{2}\right)-\sum_{i=1}^{n}e_i-m+\sum_{i=1}^{n}\sum_{j=1}^{e_i}\frac{1}{3-j}\right].$$

Conversely,

$$\begin{aligned}RCDN(v_i\,|\,G)&=\sum_{j=1}^{n}\frac{1}{1+D-d(v_i,v_j)}\\&=\sum_{v_j\in A_1(v_i)}\frac{1}{1+D-d(v_i,v_j)}+\sum_{v_j\in A_2(v_i)}\frac{1}{1+D-d(v_i,v_j)}+\\&\quad\sum_{v_j\in A_3(v_i)}\frac{1}{1+D-d(v_i,v_j)}\end{aligned}\tag{8}$$

The first summation of Eq. (8) contains the distance between v_i and the vertices on its eccentric path $P(v_i)$. Second summation of Eq. (8) contains the distance between v_i and its neighbor which are not on the eccentric path $P(v_i)$. The third summation of Eq. (8) contains the distance between v_i and a vertex which is neither adjacent to v_i nor on the eccentric path $P(v_i)$. Hence the equality in Eq. (8) holds if and only if $D \le 2$. It is true for all $v_i \in V(G)$, which completes the proof. □

Corollary 6. Let G be a self-centered graph with n vertices and radius $r = r(G)$. Then

$$RCW(G)\le\frac{1}{2}\left[n^2-nr-2m+\frac{2m-n}{r}+n\sum_{j=1}^{e_i}\frac{1}{r-(j-1)}\right].$$

Equality holds if and only if $D \le 2$.

Proof. Follows by substituting $e_i = e(v_i) = r$, for $i = 1, 2, \ldots, n$ in Theorem 5. □

Algorithm: To compute RCW index

Distance matrix of a graph G is a matrix $Dt(G) = [d_{ij}]$ of order n, where $d_{ij} = d(v_i, v_j)$.

Input: Distance matrix of a given graph.

Step 1: Declared d[i] [j], *rc* [i] [j], $D = 0$, $RCW = 0$, Sum = 0.

Step2: Read the distance matrix of order n.

Step 3: For $i \rightarrow 1$ to n

For $j \rightarrow 1$ to n

if (*d*[i] [j] >*D*)

$D \rightarrow$ *d*[i] [j].

Step 4: For $i \rightarrow 1$ to n

For $j \rightarrow 1$ to n

Set *rc*[i] [j] = 0 if $i = j$ and *rc*[i][j] = $1/(1+D - d_{ij})$, otherwise.

Sum= Sum + *rc*[i] [j].

Step 5: Compute *RCW* = Sum divided by 2.

Step 6: Display *RCW*.

Output: *RCW* index of given graph.

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The F–Index for some Special Graphs and some Properties of the F–Index

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ABSTRACT

The "forgotten topological index" or "F–index" has been introduced by Furtula and Gutman in 2015. The F–index of a (molecular) graph is defined as the sum of cubes of the vertex degrees of the graph. In this paper, we compute this topological index for some special graphs such as Wheel graph, Barbell graph and friendship graph. Moreover, the effects on the F–index are observed when some operations such as edge switching, edge moving and edge separating are applied to the graphs. Finally, we investigate degeneracy of F–index for small graphs.

1 INTRODUCTION

Throughout this paper, we only consider finite, connected, undirected and simple graphs. Let G be such a graph with the vertex set $V(G)$ and the edge set $E(G)$. For a vertex $u \in V(G)$, $d_G(u)$ denotes the degree of u which is the number of edges incident to u and $N_G(u)$ is neighbor vertex set of u. Clearly $d_G(u) = |N_G(u)|$. The maximum degree of vertices in G is denoted by $\Delta(G)$. For a subset W of $V(G)$, let $G - W$ be the subgraph of G obtained by deleting the vertices of W together with their incident edges. Similarly, for a subset E' of $E(G)$, we denote by $G - E'$ the

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subgraph of G obtained by deleting the edges of E'. If $W = \{u\}$and $E' = \{xy\}$, the subgraphs $G - W$ and $G - E'$ will be written as $G - u$ and $G - xy$ for short, respectively. For any two nonadjacent vertices x and y of graph G, we let $G + xy$ be the graph obtained from G by adding an edge xy. As usual, let C_n and K_n be the cycle and complete graph on n vertices, respectively.

Chemical graph theory is a branch of mathematical chemistry where molecular structures are modeled as molecular graphs. A molecular graph is a simple unweighted, undirected graph where the vertices correspond to the atoms in the molecule and the edges correspond to the covalent bonds between them. A single number, representing a chemical structure, in graph – theoretical terms, is called a *topological descriptor*. It must be a structural invariant, i.e., it does not depend on the labeling or the pictorial representation of a graph. If such a topological descriptor correlates with a molecular property, it is named *molecular index* or *topological index*. In fact, a topological index is numeric quantity derived from a molecular graph which correlates with the physico–chemical properties of the molecule. Different topological indices are used for quantitative structure–property relationship **(QSPR)** and quantitative structure–activity relationship **(QSAR)** [8,9,17,25].

In [15], Gutman and Trinajstić introduced the most famous vertex – degree based topological indices and named them as the *first Zagreb index* and *second Zagreb index*. These topological indices were elaborated in [14]. For a (molecular) graph G, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$of G are defined as follows:

$$M_1(G) = \sum_{v\in V(G)} d_G(v)^2 \ \& M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v).$$

The first Zagreb index can also expressed as [10]:

$$M_1(G) = \sum_{uv\in E(G)}[d_G(u) + d_G(v)].$$

For more information on the Zagreb indices and their applications see [3, 4, 18, 24, 25, 28].

Gutman and Trinajstić in [15] obtained the approximate formulas for the total π–electron energy. In these formulas, there was the sum of the cubes of the degrees of all vertices of the molecular graph. This sum, except in a few works about the general first Zagreb index [20,21] and the zeroth – order general Randić index [16], has been completely neglected. Recently, Furtula and Gutman named this sum as "*forgotten topological index*" [11] and they studied some basic properties of this index. The forgotten topological index, or shortly the "*F–index*" $F(G)$ of a (molecular) graph G is defined as:

$$F(G) = \sum_{v\in V(G)} d_G(v)^3.$$

We can rewrite the F–index as [10]:

$$F(G) = \sum_{uv\in E(G)}[d_G(u)^2 + d_G(v)^2].$$

For more information on the F–index see [1, 2, 5, 6, 12, 13, 27].

In papers [2, 6, 12, 27], the authors computed the F–index for some special graphs and in papers [1,5,13], the authors presented some properties of the F–index. These motivate us to compute the F–index for some other special graphs and present some other properties of the F–index.

In this paper, we compute the F–index for some special graphs such as Wheel graph, Barbell graph and Friendship graph [23]. Moreover, the effects on this index are observed when some operations such as edge switching, edge moving and edge separating [22] are applied to the graphs. Finally, we investigate degeneracy the F–index for small graphs.

2. THE F–INDEX FOR SOME SPECIAL GRAPHS

2.1. WHEEL GRAPH

A Wheel graph is a graph with p vertices, formed by connecting a single vertex to all vertices of C_{p-1}. It is denoted as W_p [23]. Graphs W_4, W_5, W_6,W_7, W_8 and W_9 are shown in Figure 1.

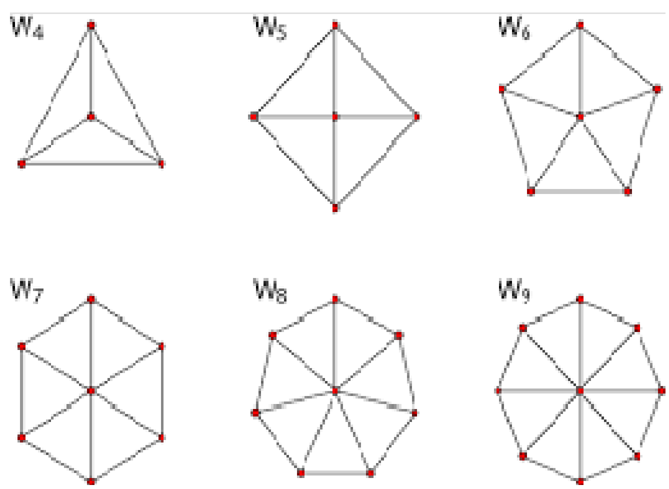

Figure 1. Graphs W_4, W_5, W_6,W_7, W_8 and W_9.

Wheel graphs are planar graphs and as such have a unique planar embedding. They are self–dual, the planar dual of any Wheel graph is an isometric graph. Any maximal planar graph, other than $K_4 = W_4$, contain as a subgraph either W_5 or W_6. There is always a Hamiltonian cycle in the Wheel graph and there are $(p^2 - 3p + 3)$ cycles in W_p [23].

Theorem 2.1. Let W_p be the Wheel graph with p vertices, $p \geq 4$, then its F–index is equal to $F(W_p) = (p-1)(p^2 - 2p + 28)$.

Proof. From the construction of Wheel graph W_p, it is clear that graph W_p has $p-1$ vertices with degree 3 and 1 vertex with degree $p-1$. Hence we have:

$$F(W_n) = \sum_{v \in V(W_p)} d_{W_p}(v)^3 = (p-1)(3)^3 + 1(p-1)^3$$
$$= (p-1)(p^2 - 2p + 28).$$

□

2.2. BARBELL GRAPH

A p–Barbell graph is the simple graph obtained by connecting two copies of a complete graph K_p by a bridge and it is denoted by B_p [23]. Graphs B_3, B_4, B_5 and B_6 are shown in Figure 2.

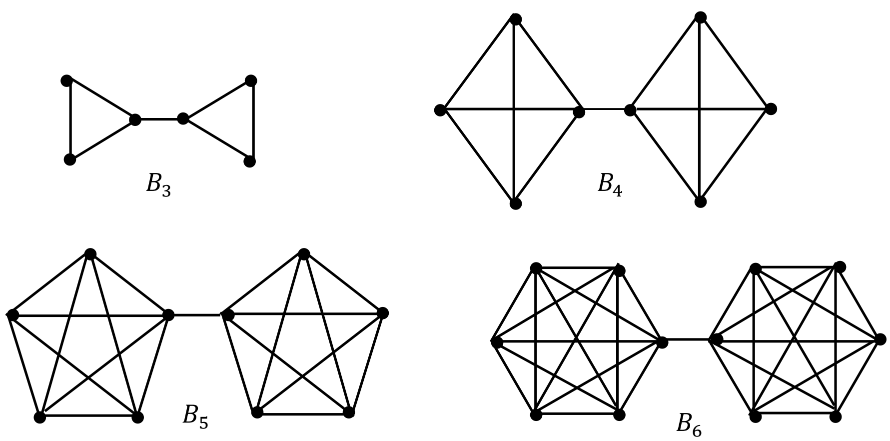

Figure 2. Graphs B_3, B_4, B_5 and B_6.

Theorem 2.2. Let B_p be the p – Barbell graph where $p \geq 3$, then its F–index is equal to $F(B_p) = 2[(p-1)^4 + p^3]$.

Proof. From the construction of graph B_p, it is clear that graph B_p has $2p-2$ vertices with degree $p-1$ and 2 vertices with degree p. Hence we have:

$$F(B_p) = \sum_{v \in V(B_p)} d_{B_p}(v)^3 = (2p-2)(p-1)^3 + 2p^3 = 2[(p-1)^4 + p^3].$$

□

2.3. FRIENDSHIP GRAPH

A p – Friendship graph is the simple graph obtained by joining p copies of C_3 with a common vertex and it is denoted as F_p [23]. $F_p$is a planar undirected graph with $2p + 1$ vertices and $3p$ edges. Graphs F_2, F_3 and F_4 are shown in Figure 3.

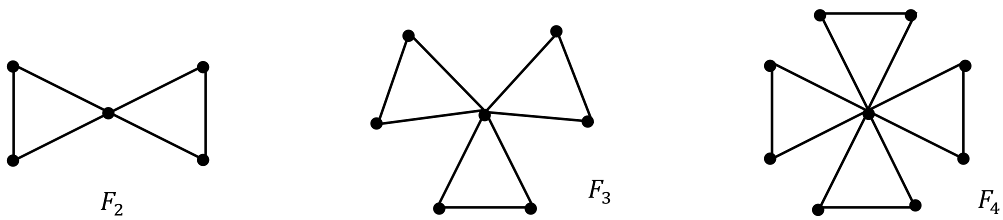

Figure 3. Graphs F_2, F_3 and F_4.

Theorem 2.3. Let F_p be the p–friendship graph, $p \geq 2$, then its F–index is equal to $F(F_p) = 8p(p^2 + 2)$.

Proof. From the construction of graph F_p, it is clear that graph F_p has $2p$ vertices with degree 2 and 1 vertex with degree $2p$. Hence we have:

$$F(F_p) = \sum_{v \in V(F_p)} d_{F_p}(v)^3 = 2p(2)^3 + 1(2p)^3 = 8p(p^2 + 2).$$

□

3. SOME PROPERTIES OF THE F–INDEX

Proposition 3.1. Let G be a connected graph with two nonadjacent vertices $u, v \in V(G)$ and $G' = G + uv$. Then we have:

$$F(G') = F(G) + 2 + 3(d_G(u)^2 + d_G(u) + d_G(v)^2 + d_G(v)).$$

Proof. By the definition of the F–index, we have:

$$\begin{aligned} F(G') - F(G) &= (d_{G'}(u)^3 + d_{G'}(v)^3) - (d_G(u)^3 + d_G(v)^3) \\ &= (d_G(u) + 1)^3 - d_G(u)^3 + (d_G(v) + 1)^3 - d_G(v)^3 \\ &= 2 + 3(d_G(u)^2 + d_G(u) + d_G(v)^2 + d_G(v)), \end{aligned}$$

which completes the proof. □

From Proposition 3.1, we have the following corollary.

Corollary 3.1. If u and v are two nonadjacent vertices in graph G, then we have:

$$F(G + uv) > F(G).$$

3.1. EDGE SWITCHING OPERATION

Theorem 3.1.1. Let u and v be two nonadjacent vertices of a connected graph G with $d_G(u) \geq d_G(v)$. Suppose $v_1, v_2, \ldots, v_s \in N_G(v) \setminus N_G(u), 1 \leq s \leq d_G(v)$. Let $G^* = G - \{vv_1, vv_2, \ldots, vv_s\} + \{uv_1, uv_2, \ldots, uv_s\}$, then $F(G^*) > F(G)$.

Proof. By the definition of the F–indexand the construction of graph G^*, we have:

$$\begin{aligned} F(G^*) - F(G) &= (d_{G^*}(u)^3 + d_{G^*}(v)^3) - (d_G(u)^3 + d_G(v)^3) \\ &= (d_G(u) + s)^3 - d_G(u)^3 + (d_G(v) - s)^3 - d_G(v)^3 \\ &= 3s(d_G(u)^2 - d_G(v)^2) + 3s^2(d_G(u) + d_G(v)) > 0. \end{aligned}$$

The last inequality follows from $d_G(u) \geq d_G(v)$. Therefore, $F(G^*) > F(G)$. □

Theorem 3.1.2. Let $\mathcal{G}_{n,m}$ be the set of connected graphs of order n and size m.Suppose $G \in \mathcal{G}_{n,m}$ with maximum F–index, then we have $\Delta(G) = n - 1$.

Proof. If $\Delta(G) = n - 1$, our result in this theorem holds immediately. If not, we choose a vertex u in the graph G with maximum degree and another vertex $v \in V(G)$ such that u is not adjacent to v. So we have $d_G(u) \geq d_G(v)$. Assume that $N_G(v) \setminus N_G(u) = \{v_1, v_2, \ldots, v_s\}$. Note that $N_G(v) \setminus N_G(u) \neq \emptyset$ because of the fact that $d_G(u) < n - 1$. Now we construct a new graph G^* as:

$$G^* = G - \{vv_1, vv_2, \ldots, vv_s\} + \{uv_1, uv_2, \ldots, uv_s\}.$$

From Theorem 3.1.1, we have $F(G^*) > F(G)$. Thus we find that $G^* \in \mathcal{G}_{n,m}$ with a larger F–index than that of G. This is a contradiction to the choice of G, which finishes the proof of this theorem. □

3.2. EDGE MOVING OPERATION

Suppose v is a vertex of graph G. As shown in Figure 4. Let $G_{k,l}$ $(1 \leq k \leq l)$ be the graph obtained from G by attaching two new paths $P: v(= v_0)v_1v_2 \ldots v_k$ and $Q: v(= u_0)u_1u_2 \ldots u_l$ of length $k$and l, respectively, at v, where $v_1, v_2, \ldots, v_k$ and $u_1, u_2, \ldots, u_l$ are distinct new vertices. Let $G_{k-1,l+1} = G_{k,l} - v_{k-1}v_k + u_lv_k$.

Theorem 3. 2. Let G be a connected graph of order $n \geq 2$ and $1 \leq k \leq l$**.**

(1) If $k \geq 2$, then $F(G_{k,l}) = F(G_{k-1,l+1})$.

(2) $F(G_{1,l}) > F(G_{0,l+1})$.

Proof (1). By the definition of the F–index and the construction of graph $G_{k,l}$, we have:

$$\begin{aligned} F(G_{k,l}) - F(G_{k-1,l+1}) &= \left(d_{G_{k,l}}(v_{k-1})^3 + d_{G_{k,l}}(v_k)^3 + d_{G_{k,l}}(u_l)^3\right) \\ &\quad -\left(d_{G_{k-1,l+1}}(v_{k-1})^3 + d_{G_{k-1,l+1}}(u_l)^3 + d_{G_{k-1,l+1}}(v_k)^3\right) \\ &= (2^3 + 1^3 + 1^3) - (1^3 + 2^3 + 1^3) \\ &= 0, \end{aligned}$$

which completes the Proof of (1).

Proof (2).

$$\begin{aligned} F(G_{1,l}) - F(G_{0,l+1}) &= \left(d_{G_{1,l}}(v_1)^3 + d_{G_{1,l}}(v)^3 + d_{G_{1,l}}(u_l)^3\right) \\ &\quad -\left(d_{G_{0,l+1}}(v)^3 + d_{G_{0,l+1}}(u_l)^3 + d_{G_{0,l+1}}(v_1)^3\right) \\ &= \left(1^3 + \left(d_{G_{0,l+1}}(v) + 1\right)^3 + 1^3\right) \\ &\quad -\left(d_{G_{0,l+1}}(v)^3 + 2^3 + 1^3\right) \\ &= \left(3d_{G_{0,l+1}}(v)^2 + 3d_{G_{0,l+1}}(v) + 1^3 + 1^3\right) - (2^3) > 0\,. \end{aligned}$$

Note that G is a connected graph with $n \geq 2$ vertices, so then $d_{G_{0,l+1}}(v) \geq 2$. Hence the last inequality follows easily. Therefore, $F(G_{1,l}) > F(G_{0,l+1})$. $\square$

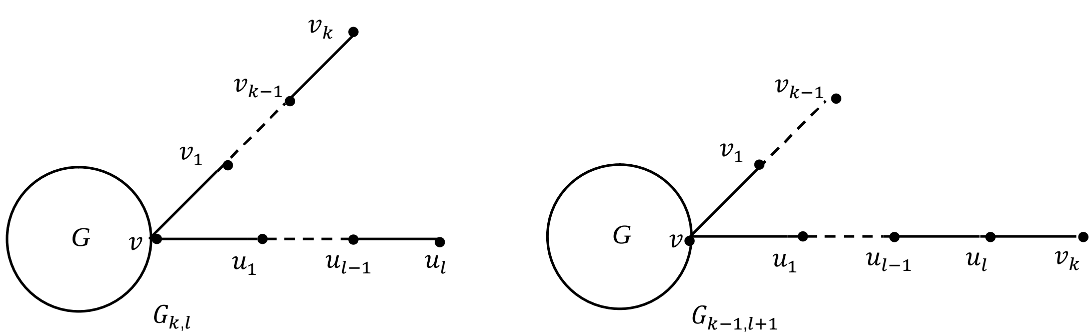

Figure 4.

3.3. EDGE SEPARATING OPERATION

Let $e = uv$ be a cut edge of a graph G. If G' is obtained from G by contracting the edge e into a new vertex u_e, which becomes adjacent to all the former neighbors of u and of v, and adding a new pendent edge $u_e v_e$, where v_e is a new pendent vertex. We say that G' is obtained from G by separating an edge uv (see Figure 5).

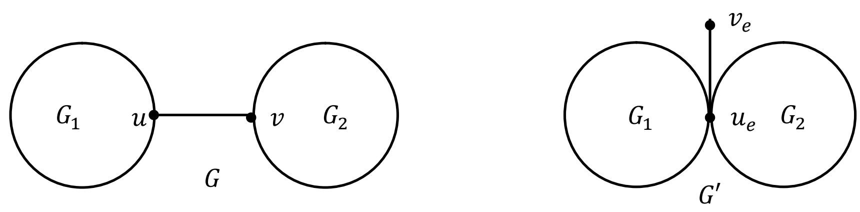

Figure 5.

Theorem 3.3. Let $e = uv$ be a cut edge of a connected graph G, where $d_G(u) \geq 2$ and $d_G(v) \geq 2$. Suppose G' is the graph obtained from G by separating the edge uv. Then $F(G') > F(G)$.

Proof: By the definition of the F–index and the construction of graph G', we have:

$$F(G') - F(G) = [d_{G'}(u_e)^3 + d_{G'}(v_e)^3] - [d_G(u)^3 + d_G(v)^3]$$
$$= [(d_G(u) + d_G(v) - 1)^3 + 1^3] - [d_G(u)^3 + d_G(v)^3]$$
$$-[d_G(u)^3 + d_G(v)^3]$$
$$= \left[\left(d_G(u) + d_G(v)\right)^3 - 3\left(d_G(u) + d_G(v)\right)^2 + 3\left(d_G(u) + d_G(v)\right)\right]$$
$$= 3(d_G(u) + d_G(v))(d_G(u)d_G(v) + 1) - 3\left(d_G(u) + d_G(v)\right)^2 > 0.$$

Since $d_G(u) \geq 2$and $d_G(v) \geq 2$, so then $d_G(u)d_G(v) \geq d_G(u) + d_G(v)$. Hence the last inequality follows easily. Therefore, $F(G') > F(G)$. □

3.4. k – APEX TREES

A tree is a connected acyclic graph. For any positive integer k with $k \geq 1$, a graph G is called a k – apex tree if there exists a subset X of $V(G)$ such that $G - X$ is a tree and $|X| = k$, while for any $Y \subseteq V(G)$ with $|Y| < k$, $G - Y$ is not a tree. A vertex of X is called a k – apex vertex [26]. For positive integers $n \geq 3$ and $k \geq 1$, let $\mathbb{T}(n, k)$ denote the class of all k – apex trees of orden n.

Theorem 3.4. Let $G \in \mathbb{T}(n, k)$ and v be a k – apex vertex of G. If $F(G)$ is maximum in $\mathbb{T}(n, k)$, then $d_G(v) = n - 1$.

Proof. Since $G \in \mathbb{T}(n, k)$, we have $|V(G)| = n$. Hence $d_G(u) \leq n - 1$ for all $u \in V(G)$. Suppose that $d_G(v) \neq n - 1$, so then $d_G(v) < n - 1$. Then there exists a vertex u in G such that $uv \notin E(G)$. Then by Corollary 3.1, we have $F(G +$

$uv) > F(G)$. Clearly $G + uv \in \mathbb{T}(n,k)$ and it contradicts to that $F(G)$ is maximum in $\mathbb{T}(n,k)$. Therefore, $d_G(v) = n-1$. □

Proposition 3.4. Let $G \in \mathbb{T}(n,k)$. If $F(G)$ is maximum in $\mathbb{T}(n,k)$, then we have:

$$|E(G)| = \frac{k(2n-k-3)}{2} + n - 1 .$$

Proof. Let X be the set of all k – apex vertices in G. Then $|X| = k$. Since $F(G)$ is maximum in $\mathbb{T}(n,k)$, then by Theorem 3.4, we have $d_G(v) = n-1$ for all $v \in X$ Hence the subgraph induced by X is a complete graph of order k and $G - X$ is a tree of order $n-k$. Thus

$$|E(G)| = \binom{k}{2} + k(n-k) + (n-k-1) = \frac{k(2n-k-3)}{2} + n - 1.$$

□

3.5. Line Graph

The line graph, $L(G)$, of a graph G has the vertex set $V\big(L(G)\big) = E(G)$ and two distinct vertices of $L(G)$ are adjacent if the corresponding edges of G share a common end vertex. The iterated line graph, $L^k(G)$, of G is defined as $L^k(G) = L(L^{k-1}(G))$, where $k \geq 1$ and $L^0(G) \cong G$. What we can say about values of the index with increasing k? We consider the case of r-regular graphs G, $r \geq 3$. Denote by r_k and n_k the degree and the order of $L^k(G)$, respectively. It is not hard to calculate that $r_k = 2^k(r-2) + 2$ and $n_k = \frac{1}{2^k} n \prod_{i=0}^{k-1} r_i$. Then $F(L^k(G)) = \frac{1}{2^k} n(2^k(r-2)+2)^3 \prod_{i=0}^{k-1}(2^i(r-2)+2)$. For example, the third line iteration of cubic graph G of order $n$gives $F\big(L^3(G)\big) = 9000n$.

4. Degeneracy the F–Index for Small Graphs

A topological index is called degenerate if it possesses the same value for more than one graph. A set of graphs with the same value of a given index forms a degeneracy class. Since a topological index can be regarded as a measure of structural similarity of molecular graphs, the finding of information on degeneracy classes can be useful for chemical applications. There are a number of functions for characterizing degeneration of topological indices [7]. The discriminating ability of an index for a family of graphs can be expressed by relation

{number of unique values of an index} / {number of the considered graphs}.

The number of unique values, of course, coincides with the number of degeneracy classes. The similar measure was introduced in [19] where the number of trivial degeneracy classes was used. Table 1 contains comparative data for trees, unicyclic and bicyclic graphs of small order. One can see that the discriminating ability of F-index is between discriminating ability of indices M_1 and M_2.

n	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
	Trees																
M_1	1	1	.83	.64	.39	.28	.17	.09	.05	.03	.01	.006	.003	.001	.001	.000	.000
F	1	1	.83	.64	.49	.32	.19	.12	.08	.04	.02	.011	.006	.003	.001	.001	.000
M_2	1	1	1	.82	.74	.47	.33	.18	.10	.05	.03	.013	.007	.003	.001	.001	.000
	Unicyclic Graphs																
M_1	1	.8	.46	.27	.17	.07	.03	.014	.007	.003	.001	.001	.000	.000			
F	1	.8	.54	.33	.18	.01	.05	.024	.012	.006	.003	.001	.000	.000			
M_2	1	1	.77	.55	.30	.16	.08	.038	.017	.007	.003	.001	.001	.000			
	Bicyclic Graphs																
M_1	1	.6	.32	.15	.06	.024	.009	.004	.001	.000	.000						
F	1	.8	.47	.21	.09	.039	.017	.007	.003	.001	.000						
M_2	1	1	.74	.36	.16	.063	.025	.010	.004	.001	.000						

Table 1. Discriminating ability of indices for small n-vertex graphs.

Examples of trees of order 10, unicyclic graphs of order 11, and bicyclic graphs of order 13 for which these three indices coincide are presented in Figure 6. We have $F(T_1) = M_1(T_2) = M_2(T_3) = 66$, $F(G_1) = M_1(G_2) = M_2(G_3) = 88$, and $F(G_4) = M_1(G_5) = M_2(G_6) = 142$.

5. CONCLUSION

Topological indices are designed basically by transforming a molecular graph into a number. The "forgotten topological index" (F–index) was introduced recently by B. Furtula and I. Gutman in 2015 [11]. In this paper, we computed the F–index for some special graphs such as wheel graph, Barbell graph and Friendship graph. Moreover, the effects on the F–index were observed when some operations such as edge switching, edge moving and edge separating were applied to the graphs. However, there are still many other special graphs and operations which are not covered here. So, for further studies, F–index of some other special graph can be computed and also properties of the F–index under some other operations can be investigated.

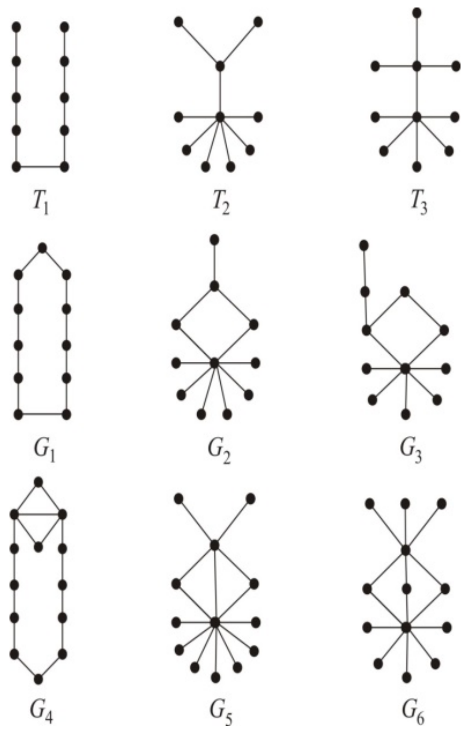

Figure 6. Graphs with the same indices.

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On the Bicyclic Graphs with Minimum Reduced Reciprocal Randić Index

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ABSTRACT

The reduced reciprocal Randić (RRR) index is a molecular structure descriptor (or more precisely, a topological index), which is useful for predicting the standard enthalpy of formation and normal boiling point of isomeric octanes. In this paper, a mathematical aspect of RRR index is explored, or more specifically, the graph(s) having minimum RRR index is/are identified from the collection of all n–vertex connected bicyclic graphs for $n \geq 5$. As a consequence, the best possible lower bound on the RRR index, for n–vertex connected bicyclic graphs is obtained when $n \geq 5$.

1 INTRODUCTION

It is widely known fact that a graph can be used to represent a molecule in which atoms correspond to the vertices while the molecular bonds between atoms represent edges [1, 5]. In chemical graph theory, those graph invariants are usually referred as topological indices which are expected to correlate with some physical observable measures by experiments in such a way that theoretical predictions can be used to gain chemical insights even for not yet existing molecules [2]. Applications of topological indices in chemistry begin in 1947, when the chemist

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Wiener [6] devised a topological index, nowadays known as Wiener index, for predicting the boiling points of paraffins.

All graphs considered in this paper are simple and finite. Undefined notations and terminologies from (chemical) graph theory can be found in [1-4].

The Randić index [7] is one of the most studied and most applied topological indices, which was proposed in 1975 for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. The Randić (R) index for a graph G is defined as

$$R(G) = \sum_{uv\in E(G)} (d_u d_v)^{-\frac{1}{2}},$$

where uv is the edge connecting the vertices u, v of the graph G, $E(G)$ is the edge set of G and d_u is degree of the vertex u. Determining the graphs with minimum or maximum R value from certain collections of graphs with some fixed parameters, was the topic of several publications. For instance, Bollobás and Erdős [8] identified the unique tree with minimum R value among all n–vertex trees, when $n \geq 3$. The unique graph with minimum R value was determined in [9] (respectively, in [10]) from the class of all n–vertex connected unicyclic (respectively, bicyclic) graphs, when $n \geq 5$. Details about the chemical applicability and mathematical properties of R can be found in the surveys [11, 12], recent papers [13-20] and/or related references listed therein.

Based on the successful consideration of Randić index, Manso *et al.* [21] introduced a new topological index (and named it *Fi* index) to predict the normal boiling point temperatures of hydrocarbons. In the mathematical definition of *Fi* index two terms are present. In 2014, Gutman *et al.* [22] considered one of these terms, which is given below:

$$RRR(G) = \sum_{uv\in E(G)} \sqrt{(d_u - 1)(d_v - 1)},$$

and they called it *reduced reciprocal Randić* (RRR) *index*. In [22], the RRR index was compared with several well-known topological indices for predicting the standard heats (enthalpy) of formation and normal boiling points of octane isomers, and it was concluded that RRR index deserves attention of researchers performing quantitative structure-property relationship and quantitative structure-activity relationship studies.

The study of extremal graphs with respect to the RRR index was initiated by the authors of [22]. They proved that the star graph and the complete graph have the minimum and maximum value, respectively, among all n-vertex graphs, and also posed a conjecture related to the maximum RRR value of trees. This conjecture was proved by Ren *et al.* [23]. Recently, the problem of finding graph with minimum RRR value among all n-vertex connected unicyclic graphs (n-vertex connected graphs with n edges) was solved in [24]. Main purpose of the present paper is to extend the main result of the reference [24] for connected bicyclic graphs (n-vertex connected graphs with $n + 1$ edges), or more precisely, to solve the following extremal problem.

Problem 1. *Which graph(s) has/have minimum RRR index among all n-vertex connected bicyclic graphs*?

As there is only one bicyclic graph on 4 vertices, so the Problem 1 is well defined for $n \geq 5$ and thereby in the remaining part of this paper, it would be assumed that the graph under consideration has at least 5 vertices.

Nowadays, many researchers are interested in finding best possible bounds on topological indices; for example, see [25-29]. As a consequence of our main result, we obtain best possible lower bound on the RRR index, for n–vertex connected bicyclic graphs when $n \geq 5$.

2. MAIN RESULTS

In order to prove the main result, we need some definitions. If $uv, vw \in E(G)$ but $uw \not\in E(G)$, then the vertex v and the vertex w will be called *first neighbor* of u and *second neighbor* of u, respectively. Denote by $N_G(u)$ (or simply by $N(u)$) the set of all first neighbors of u in G. The minimum and maximum degree of G will be denoted by $\delta(G)$ and $\Delta(G)$, respectively. A vertex with degree one is known as a pendent vertex. Now, we are in a position to prove the main result, which gives the complete solution of Problem 1.

Theorem 1. *Among all n–vertex connected bicyclic graphs,*

- $\tilde{B}_n$ *is the only graph with minimum RRR value for* $5 \leq n \leq 9$*;*
- $\hat{B}_n$ *is the only graph with minimum RRR value for* $10 \leq n \leq 13$*;*
- $\hat{B}_n$ *and* B'_n *are the only graphs with minimum RRR value for* $n = 14$*;*
- B'_n *is the only graph with minimum RRR value for* $n \geq 15$*, where the graphs* $\tilde{B}_n$, $\hat{B}_n$ and B'_n are depicted in Figure 1.

Proof. We note that there are only five non-isomorphic connected bicyclic graphs on 5 vertices. These graphs, together with their RRR index, are depicted in Figure 2. Hence, the result is true for $n = 5$.

Now, we assume that B_n is an n-vertex connected bicyclic graph for $n \geq 6$. If $\Delta(B_n) = n - 1$, then B_n must be isomorphic to one of the graphs $B_n^{(1)}$, $B_n^{(2)}$, shown in Figure 3.

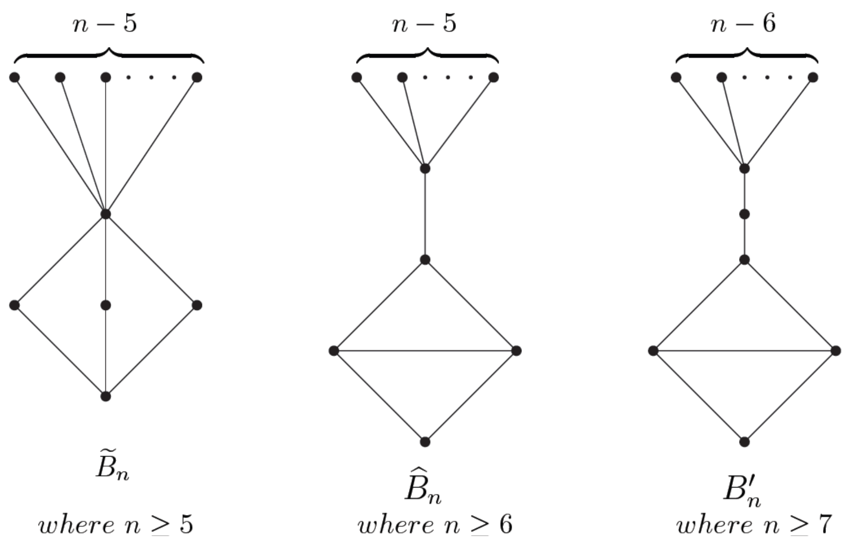

Figure 1. The graphs $\widetilde{B}_n$, $\widehat{B}_n$ and B'_n.

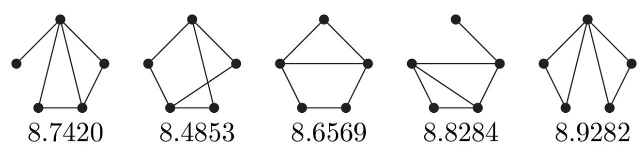

Figure 2. All the non-isomorphic connected bicyclic graphs on 5 vertices together with their RRR index.

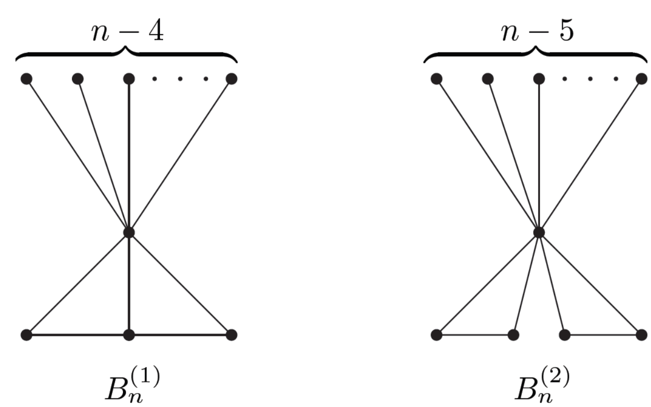

Figure 3. The graphs $B_n^{(1)}$ and $B_n^{(2)}$.

Routine calculations yield

$$RRR\left(B_n^{(1)}\right) = (2+\sqrt{2})\sqrt{n-2} + 2\sqrt{2}$$

and

$$RRR\left(B_n^{(2)}\right) = 4\sqrt{n-2} + 2.$$

Simple comparison gives

$$RRR\left(B_n^{(j)}\right) > \begin{cases} 3\left(\sqrt{n-3}+\sqrt{2}\right) = RRR\left(\tilde{B}_n\right) & for\ \ 6 \le n \le 9, \\ \sqrt{2}\left(\sqrt{n-5}+2\right)+6 = RRR\left(\hat{B}_n\right) & for\ \ 10 \le n \le 13, \\ 5\sqrt{2}+6 = RRR\left(\hat{B}_{14}\right) = RRR\left(B'_{14}\right) & for\ \ n = 14, \\ \sqrt{n-6}+3\left(2+\sqrt{2}\right) = RRR\left(B'_n\right) & for\ \ n \ge 15, \end{cases}$$

where $j = 1,2$. Now, we suppose that $\Delta(B_n) \le n-2$ where $n \ge 6$. If B_n does not contain any pendent vertex, then B_n must be isomorphic to one of the graphs $B_n^{(3)}$, $B_n^{(4)}$, depicted in Figure 4. It holds that

$$RRR\left(B_n^{(3)}\right) = \begin{cases} n+2(2\sqrt{2}-1) & if\ k = 0, \\ n+6\sqrt{2}-5 & otherwise. \end{cases}$$

and

$$RRR\left(B_n^{(4)}\right) = \begin{cases} n+4\sqrt{3}-3 & if\ q = 1, \\ n+2(2\sqrt{2}-1) & if\ q = 2, \\ n+6\sqrt{2}-5 & otherwise. \end{cases}$$

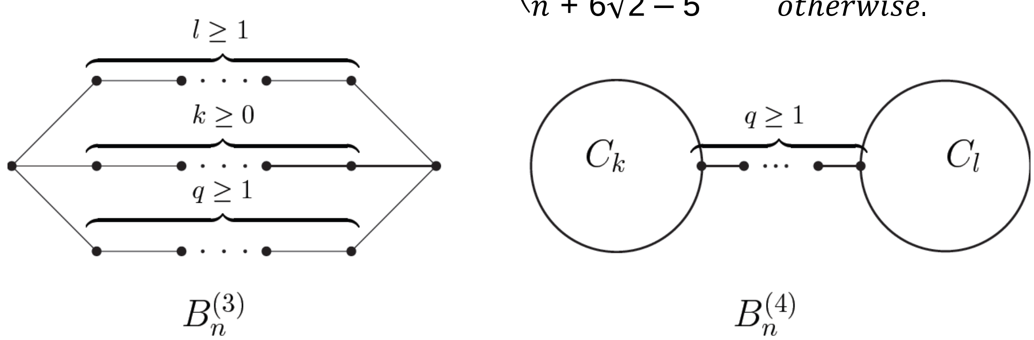

Figure 4. The graphs $B_n^{(3)}$ and $B_n^{(4)}$.

After simple comparison, we have

$$RRR\left(B_n^{(s)}\right) > \begin{cases} 3\left(\sqrt{n-3}+\sqrt{2}\right) = RRR\left(\tilde{B}_n\right) & for\ \ 6 \le n \le 9, \\ \sqrt{2}\left(\sqrt{n-5}+2\right)+6 = RRR\left(\hat{B}_n\right) & for\ \ 10 \le n \le 13, \\ 5\sqrt{2}+6 = RRR\left(\hat{B}_{14}\right) = RRR\left(B'_{14}\right) & for\ \ n = 14, \\ \sqrt{n-6}+3\left(2+\sqrt{2}\right) = RRR\left(B'_n\right) & for\ \ n \ge 15, \end{cases}$$

where $s = 3,4$. In what follows, we assume that $\delta(B_n) = 1$ and $\Delta(B_n) \le n-2$ where $n \ge 6$. Let $P(B_n) = \{u'_0, u'_1, u'_2, \ldots, u'_{p-1}\}$ be the set of all pendent vertices of B_n. For $0 \le i \le p-1$, suppose that $W_{u'_i}$ is the set of all those second neighbors of u'_i which are pendent. We choose a member of $P(B_n)$, say $u'_0 = u_0$ (without loss of generality), such that

1. the number of elements in W_{u_0} is as large as possible;
2. subject to (1), the first neighbor (say v_0) of u_0 has degree as small as possible (let $d_{v_0} = x$ and $N(v_0) = \{u_0, u_1, u_2, \ldots, u_{r-1}, u_r, \ldots, u_{x-1}\}$ where $d_{u_i} = 1$ for $0 \le i \le r-1$ and $d_{u_i} \ge 2$ for $r \le i \le x-1$);
3. subject to (1) and (2), $\sum_{i=r}^{x-1} d_{u_i}$ is as small as possible;
4. subject to (1), (2) and (3), $\max\{d_{u_r}, d_{u_{r+1}}, \ldots, d_{u_{x-1}}\}$ is as small as possible.

It is evident that $x \ge 2$. If B^*_{n-1} is the graph obtained from B_n by removing the vertex u_0, then

$$RRR(B_n) = RRR(B^*_{n-1}) + \left(\sqrt{x-1} - \sqrt{x-2}\right) \sum_{i=r}^{x-1} \sqrt{d_{u_i} - 1}. \tag{1}$$

Now, we have the following six cases: Case 1. $r \le x-3$; Case 2. $r = x-2$ and both of $d_{u_{x-2}}$ and $d_{u_{x-1}}$ are greater than 2; Case 3. $r = x-2$, one of $d_{u_{x-2}}$, $d_{u_{x-1}}$ is 2 and other is greater than 2; Case 4. $r = x-2$ and $d_{u_{x-2}} = d_{u_{x-1}} = 2$; Case 5. $r = x-1$ and $d_{u_{x-1}} > 2$; Case 6. $r = x-1$ and $d_{u_{x-1}} = 2$.

For $t = 1, 2, \ldots, 6$ and $n \ge 6$, let $\mathbb{B}_n^{(t)}$ be the collection of all those n-vertex connected bicyclic graphs which

- have at least one pendent vertex,
- have maximum vertex degree at most $n-2$ and
- fall in Case t.

Claim 1. If $B_n \in \mathbb{B}_n^{(1)}$, then $RRR(B_n) \ge 3\left(\sqrt{n-3} + \sqrt{2}\right)$ with equality if and only if $B_n \cong \tilde{B}_n$.

Proof of Claim 1. The claim will be proved by induction on n. For $n = 6$, the claim follows from Figure 5.

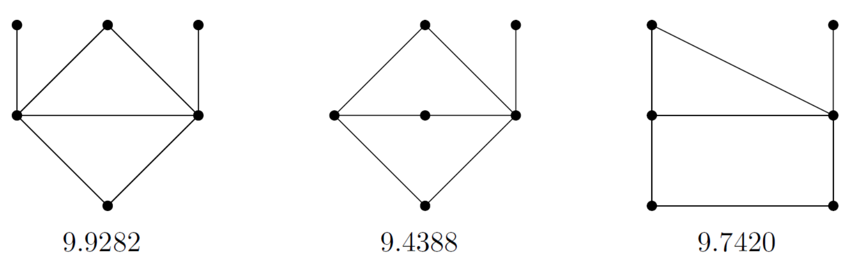

Figure 5. All the non-isomorphic members of $\mathbb{B}_6^{(1)}$ together with their RRR index.

Let us assume that $n \ge 7$. Bearing in mind the condition $r \le x-3$, inductive hypothesis and the fact $x \le n-2$, from Equation (1) we have

$$RRR(B_n) \geq RRR(\tilde{B}_{n-1}) + \left(\sqrt{x-1} - \sqrt{x-2}\right)(x-r)$$
$$\geq 3(\sqrt{2} + \sqrt{n-4}) + 3\left(\sqrt{x-1} - \sqrt{x-2}\right)$$
$$\geq 3(\sqrt{2} + \sqrt{n-4}) + 3\left(\sqrt{n-3} - \sqrt{n-4}\right) = RRR(\tilde{B}_n).$$

The equality $RRR(B_n) = RRR(\tilde{B}_n)$ holds if and only if $x = n-2, x-r = 3$ and $B_{n-1}^* \cong \tilde{B}_{n-1}$, that is $B_n \cong \tilde{B}_n$. This completes the proof of Claim 1.

Remaining claims will also be proved by induction on n.

Claim 2. If $B_n \in \mathbb{B}_n^{(2)}$, then

$$RRR(B_n) \geq \begin{cases} RRR\left(B_n^{\dagger}\right) & if \;\; n = 6, \\ RRR\left(B_n^{(5)}\right) & if \;\; n \geq 7, \end{cases}$$

where the graphs $B_n^{\dagger}$ and $B_n^{(5)}$ are shown in Figure 6. The equalities $RRR(B_6) = RRR\left(B_6^{\dagger}\right)$ and $RRR(B_n) = RRR\left(B_n^{(5)}\right)$ (for≥ 7) hold if and only if $B_6 \cong B_6^{\dagger}$ and $B_n \cong B_n^{(5)}$ respectively.

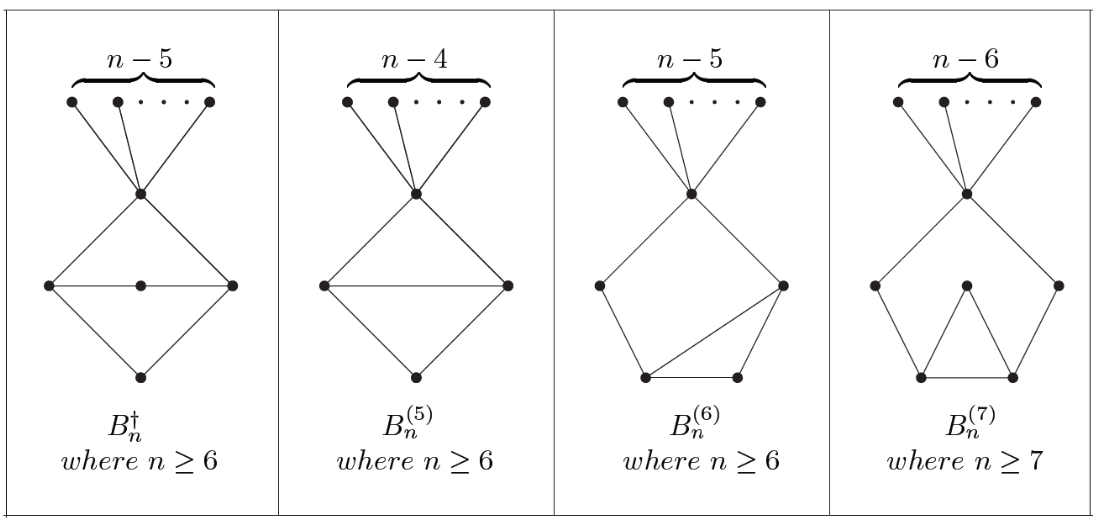

Figure 6. The graphs $B_n^{\dagger}$, $B_n^{(5)}$,$B_n^{(6)}$ and $B_n^{(7)}$.

Proof of Claim 2. For $n = 6$ and $n = 7$, the claim follows from Figures 7 and 8, respectively. Assume that $n \geq 8$. Using the inductive hypothesis in Equation (1), we get

$$\begin{aligned} RRR(B_n) &\geq RRR\left(B_{n-1}^{(5)}\right) + \left(\sqrt{x-1} - \sqrt{x-2}\right)\left(\sqrt{d_{u_{x-2}}-1} + \sqrt{d_{u_{x-1}}-1}\right) \\ &\geq 2\left[1+\sqrt{2}+\sqrt{2(n-4)}\right] + 2\sqrt{2}\left(\sqrt{x-1}-\sqrt{x-2}\right) \\ &\geq 2\left[1+\sqrt{2}+\sqrt{2(n-4)}\right] + 2\sqrt{2}\left(\sqrt{n-3}-\sqrt{n-4}\right) = RRR\left(B_n^{(5)}\right). \end{aligned}$$

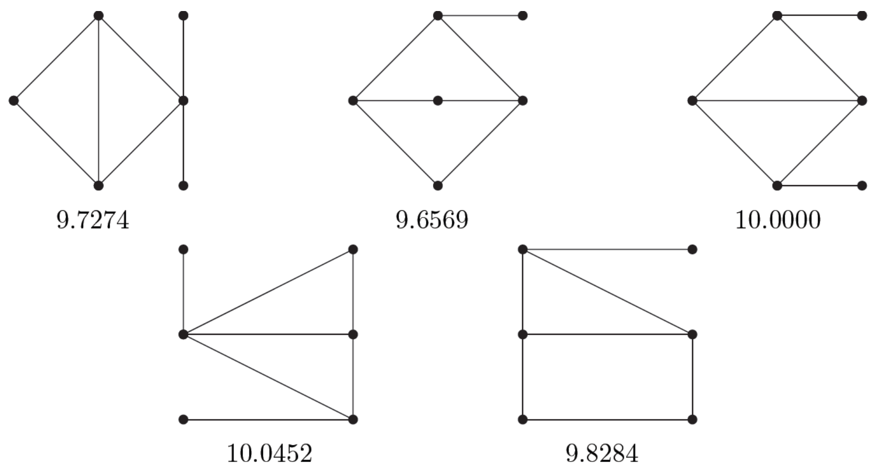

Figure 7. All the non-isomorphic members of $\mathbb{B}_6^{(2)}$ together with their RRR index.

The equality $RRR(B_n) = RRR\left(B_n^{(5)}\right)$ holds if and only if $x = n-2, d_{u_{x-1}} = d_{u_{x-2}} = 3$ and $B_{n-1}^* \cong B_{n-1}^{(5)}$.

Claim 3. If $B_n \in \mathbb{B}_n^{(3)}$, then $RRR(B_n) \geq RRR\left(B_n^{(6)}\right)$ with equality if and only if $B_n \cong B_n^{(6)}$, where the graph $B_n^{(6)}$ is shown in Figure 6.

Proof of Claim 3. The claim is obvious for $n = 6$, as Figure 9(a) suggests. Suppose that $n \geq 7$. It can be easily observed that $x \leq n-3$ because $B_n \in \mathbb{B}_n^{(3)}$. From Equation (1), it follows that

$$\begin{aligned} RRR(B_n) &\geq RRR(B_{n-1}^{(6)}) + \left(\sqrt{x-1} - \sqrt{x-2}\right)\left(\sqrt{d_{u_{x-2}}-1} + \sqrt{d_{u_{x-1}}-1}\right) \\ &\geq (1+\sqrt{2})\left(\sqrt{n-5}+\sqrt{x-1}-\sqrt{x-2}\right) + 2 + 3\sqrt{2} \\ &\geq (1+\sqrt{2})\sqrt{n-4} + 2 + 3\sqrt{2} = RRR\left(B_n^{(6)}\right). \end{aligned}$$

We note that the equality $RRR(B_n) = RRR\left(B_n^{(6)}\right)$ holds if and only if $x = n-3$, one of $d_{u_{x-2}}, d_{u_{x-1}}$ is 2 and other is 3, and $B_{n-1}^* \cong B_{n-1}^{(6)}$.

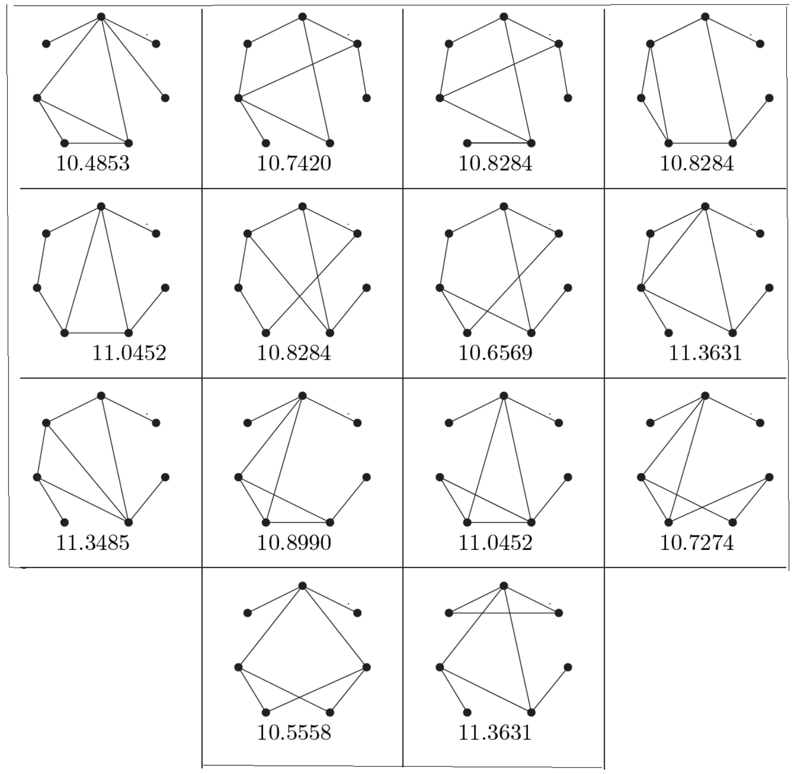

Figure 8. All the non-isomorphic members of $\mathbb{B}_7^{(2)}$ together with their RRR index.

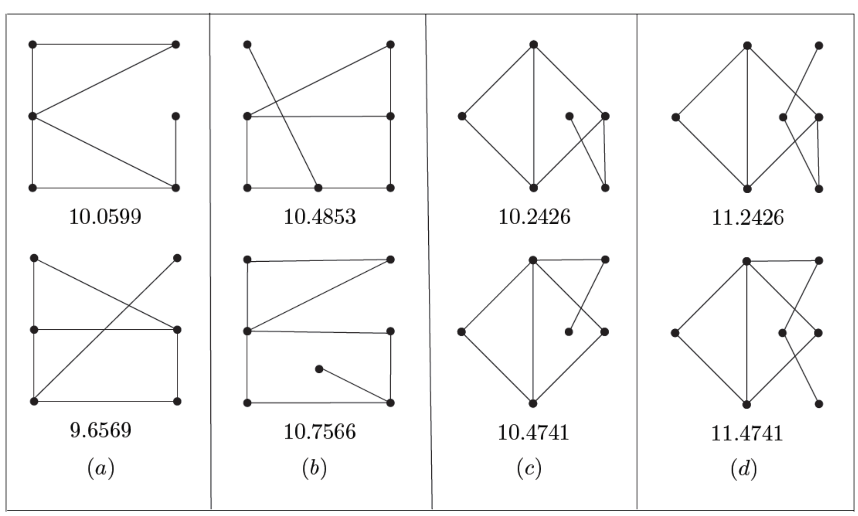

Figure 9. Parts (a), (b), (c), (d) correspond to the all non-isomorphic elements of $\mathbb{B}_6^{(3)}, \mathbb{B}_7^{(4)}, \mathbb{B}_6^{(5)}, \mathbb{B}_7^{(6)}$, respectively, together with their RRR index.

Claim 4. If $B_n \in \mathbb{B}_n^{(4)}$, then $RRR(B_n) \geq RRR\left(B_n^{(7)}\right)$ with equality if and only if $B_n \cong B_n^{(7)}$, where the graph $B_n^{(7)}$ is depicted in Figure 6.

Proof of Claim 4. We observe that the collection $\mathbb{B}_6^{(4)}$ is empty. For $n = 7$, the claim follows from Figure 9(b). Now, we assume that $n \geq 8$. It is evident that $x \leq n - 4$ as $B_n \in \mathbb{B}_n^{(4)}$. From Equation (1), it follows that

$$RRR(B_n) \geq RRR\left(B_{n-1}^{(7)}\right) + \left(\sqrt{x-1} - \sqrt{x-2}\right)\left(\sqrt{d_{u_{x-1}} - 1} + \sqrt{d_{u_{x-2}} - 1}\right)$$

$$= 2\sqrt{n-6} + 4\sqrt{2} + 2 + 2\left(\sqrt{x-1} - \sqrt{x-2}\right)$$

$$\geq 2\sqrt{n-5} + 4\sqrt{2} + 2 = RRR\left(B_n^{(7)}\right).$$

The equality $RRR(B_n) = RRR(B_n^{(7)})$ holds if and only if $x = n - 4$ and $B_{n-1}^* \cong B_{n-1}^{(7)}$.

Claim 5. If $B_n \in \mathbb{B}_n^{(5)}$, then $RRR(B_n) \geq \sqrt{2}\left(\sqrt{n-5} + 2\right) + 6$ with equality if and only if $B_n \cong \hat{B}_n$.

Proof of Claim 5. From Figure 9(c), we conclude that the claim holds for $n = 6$. Now, let $n \geq 7$. The definition of $\mathbb{B}_n^{(5)}$ guaranties that $x \leq n - 4$. Equation (1) implies that

$$RRR(B_n) \geq RRR(\hat{B}_{n-1}) + \left(\sqrt{x-1} - \sqrt{x-2}\right)\sqrt{d_{u_{x-1}} - 1}$$

$$\geq \sqrt{2}\left(\sqrt{n-6} + \sqrt{x-1} - \sqrt{x-2} + 2\right) + 6$$

$$\geq \sqrt{2}\left(\sqrt{n-5} + 2\right) + 6 = RRR(\hat{B}_n).$$

The equation $RRR(B_n) = RRR(\hat{B}_n)$ holds if and only if $x = n - 4, d_{u_{x-1}} = 3$ and $B_{n-1}^* \cong \hat{B}_{n-1}$.

Claim 6. If $B_n \in \mathbb{B}_n^{(6)}$, then $RRR(B_n) \geq RRR(B_n')$ with equality if and only if $B_n \cong B_n'$.

Proof of Claim 6. Obviously, the collection $\mathbb{B}_6^{(6)}$ is empty. For $n = 7$, the claim follows from Figure 9(d). Let us assume that $n \geq 8$. Clearly, it holds that$x \leq n - 5$ because $B_n \in \mathbb{B}_n^{(6)}$. From Equation (1), we have

$$RRR(B_n) \geq RRR(B'_{n-1}) + \left(\sqrt{x-1} - \sqrt{x-2}\right)\sqrt{d_{u_{x-1}} - 1}$$

$$= \sqrt{n-7} + 3(2 + \sqrt{2}) + \sqrt{x-1} - \sqrt{x-2}$$

$$\geq \sqrt{n-6} + 3(2 + \sqrt{2}) = RRR(B'_n).$$

The equality $RRR(B_n) = RRR(B'_n)$ holds if and only if $x = n - 5$ and $B^*_{n-1} \cong B'_{n-1}$.

For $n \geq 6$, if a graph G has minimum RRR index among all n-vertex connected bicyclic graphs then, Claims 1-6 guaranty that the graph G must belongs to the collection $\{\tilde{B}_n, B_6^{\dagger}, B_n^{(5)}, B_n^{(6)}, B_n^{(7)}, \hat{B}_n, B'_n\}$. But, the RRR index of the graphs $\tilde{B}_n, B_6^{\dagger}, B_n^{(5)}, B_n^{(6)}, B_n^{(7)}, \hat{B}_n, B'_n$ are given as

$$RRR\left(B_6^{\dagger}\right) = 4(\sqrt{2} + 1), \quad RRR(\tilde{B}_n) = 3\left(\sqrt{n-3} + \sqrt{2}\right),$$

$$RRR(\hat{B}_n) = \sqrt{2}\left(\sqrt{n-5} + 2\right) + 6, \quad RRR(B'_n) = \sqrt{n-6} + 3(2 + \sqrt{2}),$$

$$RRR\left(B_n^{(5)}\right) = 2\left(1 + \sqrt{2} + \sqrt{2(n-3)}\right),$$

$$RRR\left(B_n^{(6)}\right) = (1 + \sqrt{2})\sqrt{n-4} + 2 + 3\sqrt{2},$$

$$RRR\left(B_n^{(7)}\right) = 2\sqrt{n-5} + 4\sqrt{2} + 2.$$

After elementary comparison, we get the desired result. ∎

The following corollary is a direct consequence of Theorem 1.

Corollary 1. *For $n \geq 5$, if B_n is any n-vertex connected bicyclic graph then the following inequalities hold:*

$$RRR(B_n) \geq \begin{cases} 3\left(\sqrt{n-3} + \sqrt{2}\right) & if \;\; n \leq 9, \\ \sqrt{2}\left(\sqrt{n-5} + 2\right) + 6 & if \;\; 10 \leq n \leq 13, \\ 5\sqrt{2} + 6 & if \;\; n = 14, \\ \sqrt{n-6} + 3(2 + \sqrt{2}) & if \;\; n \geq 15. \end{cases}$$

The equality sign in the first, second and fourth inequality holds if and only if $B_n \cong \tilde{B}_n$, $B_n \cong \hat{B}_n$ and $B_n \cong B'_n$ respectively, where the graphs $\tilde{B}_n$, $\hat{B}_n$ and B'_n are depicted in Figure 1. Also, the equality sign in the third inequality holds if and only if either $B_n \cong \hat{B}_n$ or $B_n \cong B'_n$.

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ABSTRACTS
IN
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Rhombellanic Crystals and Quasicrystals

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کریستال‌ها و شبه‌کریستال‌های رمبلانی

ادیتور رابط : علیرضا اشرفی

چکیده

طرح برخی از شبکه‌های کریستال و شبه‌کریستال، بر پایهٔ کاشی‌کاری رمبلاین، ارائه شده است. پراپلاین[1,1,1] یک مولکول آلی ترکیبی است؛ فرم هیدروژنهٔ آن، پانتان[1,1,1] دوچرخه‌ای، احتمالا توسط گراف کامل دوقسمتی $K_{2,3}$ که کوچکترین رمبلاین است، نشان داده می‌شود. توپولوژی ساختارهای انتقالی و شعاعی شامل رمبلاین‌ها برحسب نماد رأس، توالی اتصال، توالی حلقه و عملیات طرح مرتبط با بذرهایشان، توصیف می‌شود. به‌وسیلهٔ مجموع تناوبی زیرساختارهای رتبه‌بندی‌شده نشان داده می‌شود که ساختارهای شعاعی، ترکیب‌های مختلط رتبهٔ بالاتر را نشان می دهند. ویژگی‌های اساسی رمبلاین ها، شامل رنگ آمیزی، مشخص می‌شوند.

لغات کلیدی: رمبلاین، کریستال، شبه‌کریستال، توپولوژی، ساختار رتبهٔ بالاتر

One–Alpha Descriptor

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توصیف‌گر یک-آلفا

ادیتور رابط : غلامحسین فتح‌تبار

چکیده

اخیرا توصیف‌گری با عنوان توصیف‌گر یک-دو تعریف شده است و نشان داده شده که پیش بینی خوبی از ظرفیت گرمایی (CP) و سطح کل (TSA) دارد. در این مقاله، تعمیم آن را با جایگزینی مقدار 2 با مقدار مثبت دلخواه α مورد تجزیه و تحلیل قرار می‌دهیم. از آنجا این توصیف‌گر می‌تواند پیش بینی‌های خوبی از CP و TSA داشته باشد، موضوع جذابی برای مطالعه است. علاوه بر این، می‌توان انتظار داشت که این توصیف‌گر در حالت کلی کاربردهای بیشتری نسبت به توصیف‌گر اولیه داشته باشد. در این مقاله، مقادیر فرینهٔ این توصیف‌گر به ازای تمام مقادیر α برای درخت‌ها به دست آمده است.

واژگان کلیدی: توصیف‌گر یک-آلفا، گراف فرینه، درخت

A new family of high-order difference schemes for the solution of second order boundary value problems

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خانواده‌ای جدید از طرحهای تفاضلی مرتبه بالا برای حل مسائل مقدار مرزی مرتبه دوم

ادیتور رابط : حسن یوسفی آذری

چکیده

مدل ریاضی بسیاری از مسائل در شیمی، نانوتکنولوژی، بیولوژی، علوم طبیعی، ریاضی-شیمی و مهندسی را می‌توان به صورت مسائل مقدار مرزی دونقطه‌ای در نظر گرفت. در حالت کلی، جواب تحلیلی برای این مسائل وجود ندارد. در این مقاله، ما یک رده از روشهای با دقت بالا برای حل حالت خاصی از مسائل مقدار مرزی دونقطه‌ای غیرخطی ارائه می‌کنیم و خطای موضعی برشی آنها مورد بحث قرار می‌گیرد. برای نشان دادن اهمیت این روشهای جدید، از آنها برای حل چند مسألهٔ معروف شامل مسألهٔ تروش، مسألهٔ براتو و برخی از مسائل منفرد خاص استفاده می‌شود. مسائل براتو و تروش در مدل‌سازی برخی از واکنشهای شیمیایی انتشار و فرایندهای انتقال حرارت رخ می‌دهند. همچنین ما نتایج حاصل از این مقاله را با برخی از نتایج موجود مقایسه کرده و نشان می‌دهیم که روشهای جدید، کارآمد و قابل اجرا هستند.

لغات کلیدی: مسألهٔ مقدار مرزی، روش‌های تفاضلات متناهی، مسألهٔ براتو، مسألهٔ تروش، دقت بالا

On Reciprocal Complementary Wiener Index of a Graph

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شاخص وینر مکمل متقابل یک گراف

ادیتور رابط : زهوئی شائو

چکیده

گریز از مرکز رأس v از G، بیشترین فاصلهٔ بین v و هر رأس دیگری در G است. شاخص وینر مکمل متقابل گراف G (RCW)، به صورت $RCW(G)=\sum_{1\le i\le j<n}\frac{1}{1+D-d(vi,vj)}$ تعریف می‌شود که D قطر G و $d(v_i,v_j)$ فاصلهٔ بین رئوس v_i و v_j است. در این مقاله، کرانهایی برای شاخص RCW بر حسب خروج از مرکزها به دست آورده‌ایم و الگوریتمی برای محاسبهٔ شاخص RCW ارائه کرده‌ایم.

لغات کلیدی: گریز از مرکز، قطر، شاخص وینر مکمل متقابل، گراف خودمحور

The F–Index for some Special Graphs and some Properties of the F–Index

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F-شاخص برای برخی از گرافهای خاص و برخی ویژگی‌های F-شاخص

ادیتور رابط : علیرضا اشرفی

چکیده

شاخص توپولوژیکی فراموش‌شده یا F- شاخص، به‌وسیلهٔ فورتالا و گوتمن در سال 2015 معرفی شده است. F- شاخص یک گراف (مولکولی) به‌صورت حاصل‌جمع مکعبات درجات رئوس یک گراف تعریف می‌شود. در این مقاله، ما این شاخص توپولوژیکی را برای برخی از گرافهای خاص از قبیل گراف چرخ، گراف هالتر و گراف دوستی محاسبه می‌کنیم. بعلاوه، تأثیرات بر F- شاخص وقتی که برخی از اعمال از قبیل تعویض یال، انتقال یال و جداسازی یال روی گرافها اعمال می‌شوند، مشاهده می شوند. سرانجام ما انحطاط F- شاخص را برای گرافهای کوچک بررسی می‌کنیم.

لغات کلیدی: شاخص توپولوژیکی فراموش‌شده، تعویض یال، انتقال یال، جداسازی یال، درخت K–نوک

On the Bicyclic Graphs with Minimum Reduced Reciprocal Randić Index

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گراف‌های دوچرخه‌ای با حداقل شاخص راندیک دوجانبهٔ کاهش‌یافته

ادیتور رابط : ایوان گوتمن

چکیده

شاخص راندیک دوجانبهٔ کاهش‌یافته (RRR)، یک توصیف کنندهٔ ساختار مولکولی (یا بطور دقیق‌تر، یک شاخص توپولوژیکی) است که برای پیش‌بینی آنتالپی استاندارد آرایش و نقطهٔ جوش نرمال اکتان‌های ایزومری مفید است. در این مقاله، جنبهٔ ریاضی شاخص RRR کشف شده است یا بطور واضح تر، گراف‌هایی که دارای حداقل شاخص RRR هستند، از مجموعهٔ همهٔ گراف‌های دوچرخه‌ای همبند n-رأسی برای $n\geq5$ شناسایی شده‌اند. بعنوان یک نتیجه، بهترین کران پایین ممکن در شاخص RRR برای گراف‌های دوچرخه‌ای همبند n- رأسی هنگامی که $n\geq5$ به‌دست آمده است.

لغات کلیدی: نظریهٔ گراف شیمیایی، توصیف‌کنندهٔ ساختار مولکولی، شاخص توپولوژیکی، شاخص راندیک دوجانبهٔ کاهش‌یافته، گراف دوچرخه‌ای

این نشریه طبق مجوز شماره 89/3/11/104372 مورخه 89/11/27 دارای اعتبار **علمی -پژوهشی** از وزارت علوم ، تحقیقات و فناوری می باشد. همچنین این مجله در پایگاه اطلاعاتی ISC (Islamic World Science Citation Center) وابسته به وزارت علوم ، تحقیقات و فناوری نمایه می شود.

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