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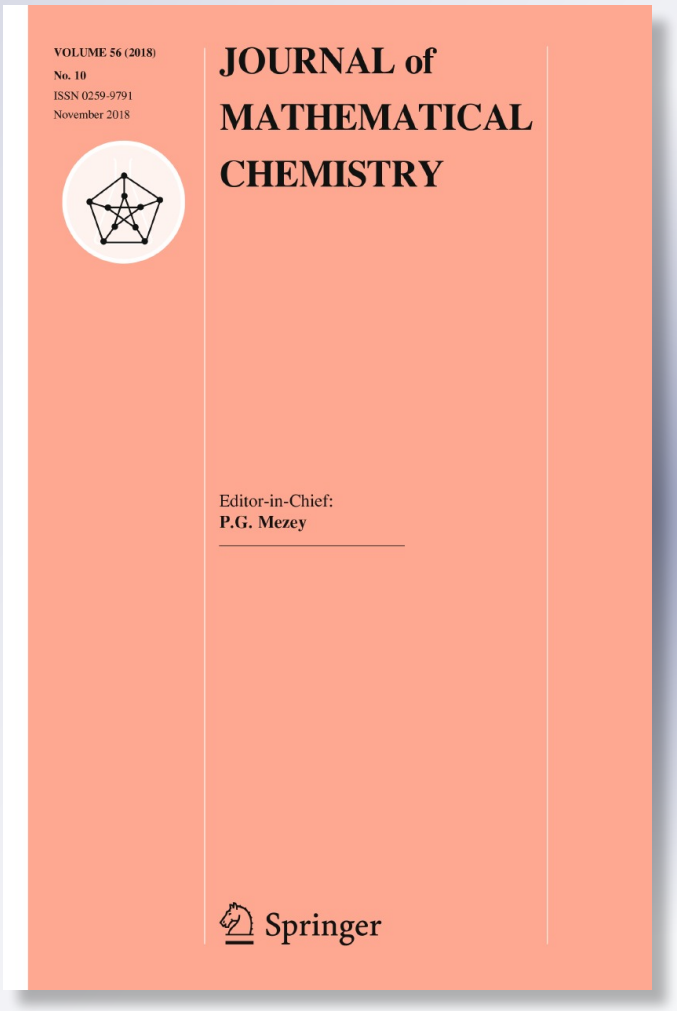

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ORIGINAL PAPER

Mostar index

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Abstract
We propose and investigate a new bond-additive structural invariant as a measure of peripherality in graphs. We first determine its extremal values and characterize extremal trees and unicyclic graphs. Then we show how it can be efficiently computed for large classes of chemically interesting graphs using a variant of the cut method introduced by Klavžar, Gutman and Mohar. Explicit formulas are presented for several classes of benzenoid graphs and Cartesian products. At the end we state several conjectures and list some open problems.

Keywords Mostar index · Peripherality · Bond-additive index

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1 Introduction

Graphs serve as models of vast number of systems whose structure and function are dependent on the connectivity pattern of their constituent elements. In order to distill and condense the information contained in connectivity patterns of graphs, a huge number of numerical quantities, variously known as structural invariants, topological descriptors, or topological indices, have been proposed and studied over the course of last decades. This phenomenon can be best observed in mathematical chemistry, in particular in the so called chemical graph theory. There the initial success of several simple invariants, such as the Wiener index [27] and the two Zagreb indices [11], motivated subsequent introduction of hundreds, if not thousands, of topological indices and their application to various chemically relevant problems [22]. Another field of successful applications of structural invariants has been the rapidly developing study of complex networks. It is interesting to observe how some invariants defined and developed within the context of chemical graph theory appear under different guises in complex networks. A nice example is the appearance of partial Wiener numbers of chemical graph theory [6] as vertex transmissions in complex networks and use of Harary index to measure global efficiency of transport networks [18].

There are many ways to define a topological index. Any procedure that produces a numerical value independent on a particular vertex labeling will result in a topological invariant. One could reasonably expect, though, that most such procedures will result in indices that are not well suited for study of interesting graph properties. Indeed, this expectation is amply empirically confirmed. Hence, one could conclude that the invariants with clear and strong structural motivation will have the best chances for successful applications.

It is reasonable to expect that interaction (if any) of two constituent elements (vertices) will be affected by their distance in the graph. This motivates introduction and study of a wide class of distance-based topological indices. Another important class is based on local properties of vertices, in particular on their degrees [4,5,10]. Yet another class of indices strives to capture some relevant properties of whole graphs by summing contributions of individual vertices and/or edges. Such indices are called vertex- and bond-additive indices, respectively [23–25].

In this paper we propose and investigate a bond-additive index that measures peripherality of individual bonds (i.e., edges) and then sums the contributions of all edges and produces a global measure of peripherality of a given graph. The basic idea is that an edge is peripheral if there are many more vertices closer to one of its end-vertices than to the other one. The most extreme case is when one of the end-vertices is a leaf, i.e., a vertex of degree one. Our proposed invariant refines in a quantitative way the idea of peripherality of edges incident with leaves. It is a bit surprising that this quantity has not been studied so far, given that its definition closely resembles definition of a common measure of graph irregularity and involves quantities that also appear in definitions of Wiener and Szeged indices.

In the next section we give the necessary definitions and place our invariant in context of previous research. In Sect. 3 we determine extremal trees and unicyclic graphs. Section 4 shows how Mostar index can be effectively computed for several classes of interesting graphs using a variant of the cut method based on Djoković–

Winkler relation Θ. Explicit formulas for various classes of benzenoid graphs and for Cartesian products of partial cubes illustrate the power of that approach. Finally, the last section states several conjectures, list some open problems, and indicates possible directions of future research.

2 Definitions and preliminary results

We first give our notation. For a given graph G, its vertex set is denoted by $V(G)$ and its edge set by $E(G)$. All graphs in this paper are simple and connected. The *degree* of a vertex $u \in V(G)$ is the number of its neighbors; we denote it by d_u. The complete graph, the path, and the star on n vertices are denoted by K_n, P_n, and S_n, respectively, while T_n denotes a generic tree on n vertices. $K_{m,n}$ denotes the complete bipartite graph with parts of sizes m and n. For terms and concepts not defined here, we refer the reader to any of classical monographs on graph theory such as, e.g., [12] or [26].

The *Wiener index* of a graph G is defined as the sum of all distances between pairs of vertices of G. Hence,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v),$$

where $d(u, v)$ denotes the usual shortest-path distance in G. For trees, $W(G)$ can be alternatively defined as

$$W(G) = \sum_{uv \in E(G)} n_u n_v,$$

where n_u denotes the number of vertices of G closer to u than to v, and n_v is defined analogously. (That was, in fact, the original definition from Ref. [27]). For general graphs, the two definitions do not coincide. However, the quantities $n_u n_v$ remain well defined for all edges of G, and their sum

$$\mathrm{Sz}\,(G) = \sum_{uv \in E(G)} n_u n_v$$

was first studied by Gutman [8]. Later it became known as the *Szeged index* of G. It has enjoyed a huge popularity among researchers in chemical graph theory and became one of discipline's success stories [9], both due to its non-trivial relationship to other topological invariants and to its intrinsic chemical interest.

Obviously, Szeged and Wiener indices coincide for trees. For graphs with cycles one always has $\mathrm{Sz}\,(G) \geq W(G)$, with equality if and only if each block of G is complete. Among all graph on n vertices, the Szeged index attains its maximum value for the balanced bipartite graph $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.

Szeged index belongs to the class of bond-additive indices. A general bond additive index is computed as a sum over all edges e of edge contributions $\phi(e)$. In case of Szeged index, $\phi(e) = n_u n_v$, where $e = uv \in E(G)$ and n_u, n_v are defined above.

There are many ways to define meaningful edge contributions, and there are many bond-additive indices. Among the best known are, certainly, the first and the second *Zagreb indices* [11], defined, respectively, by

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v) \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

For a general treatment of bond-additive indices we refer the reader to [23–25] and references therein.

In theory, contributions $\phi(e)$ of edges can be defined in any way one chooses. In practice, they are mostly given in terms of some simple functions of some quantitative properties of the end-vertices of e. When $\phi(e)$ is defined in terms of difference of some property of its end-vertices, then this contribution measures how much the end-vertices are alike. (Often the difference is taken with its absolute value to make it insensitive to the order of end-vertices.) For example, $\phi(e) = |d_u - d_v|$ measures how much the end-vertices differ in their degree. It is natural to think of the sum of all such contributions over all $e \in E(G)$ as a measure of how much G deviates from regularity. Indeed, the quantity

$$\mathrm{irr}(G) = \sum_{uv \in E(G)} |d_u - d_v|$$

has been for a long time known as the *irregularity* of G [2]. (See also [1] for a global variant.)

But what if instead of their degrees we take some other quantitative property of end-vertices of e and look at their difference? Such as, e.g., n_u and n_v? What (if anything) would be measured or quantified by so defined invariant? If this quantity is small, or even zero, it means that there are (almost) equally many vertices on both sides of e. If, on the other hand, this difference is large, it means that most, if not all, vertices lie on one side of e, and (almost) none on the other. Hence, a large value of $\phi(e) = |n_u - n_v|$ seems to indicate a peripheral position of e in G.

It seems strange that no one has looked at this quantity given its simple definition and its interpretation. (The only exceptions seem to be a fleeting mention of this quantity as the *transmission irregularity* in a recent preprint concerned with transmission-based topological indices [21] and a couple of papers concerned with *distance-balanced graphs*, for which our invariant is equal to zero; see [13,14,17,19].) Is it, maybe, because the peripherality in graphs is of no interest? Our answer is an emphatical no. After all, various measures of *centrality* dominate the research of complex networks. And any measure of peripherality could be also used to measure centrality, although the relationship is by no means trivial. Peripherality is even more important in Chemistry. It is exactly through their peripheral atoms and/or functional groups and through the corresponding bonds that molecules interact with their surroundings. Hence, it is the peripheral atoms, groups, and bonds that mostly determine their physico-chemical properties. So, we believe that it would be of interest to have a well researched and understood measure of a property that is important in several independent contexts. To this aim, we introduce a new invariant and propose to call it the *Mostar index*. The

name is chosen to honor the place of a small tri-partite workshop held in the city of Mostar in 2017 and attended by the authors. As "most" means "bridge" in both native languages of the authors, Croatian and Macedonian, and also in many others, the name also reflects the way of looking at the edge contributions: as there is no point crossing a bridge to reach a place on the same shore, there is also no point traversing an edge from one of its end-vertices to reach a vertex that is already on the same shore, i.e., closer to it than to the other end-vertex. Finally, it emphasizes the special role that cut-edges, also called bridges, play in establishing some of our results.

The *Mostar index* of a graph G is defined as

$$\mathrm{Mo}\,(G) = \sum_{e=uv \in E(G)} |n_u - n_v|.$$

For the sake of simplicity, we will often work with *contribution* $\phi(e)$ of an edge e defined as $\phi(e) = |n_u - n_v|$. The following three observations are fundamental for this measure.

Observation 1 *$\phi(e)$ has maximum value $n - 2$, and it is attained if at least one of end-vertices of e is a leaf.*

Observation 2 *$Mo\,(G) \in O(n^3)$ for a graph G on n vertices. Moreover, there are graphs with $Mo\,(G) \in \Theta(n^3)$.*

The above claim follows easily from the fact that $\phi(e) \in O(n)$ and the number of edges in the graph is $O(n^2)$. Notice that $\mathrm{Mo}\,(K_{\lfloor n/3 \rfloor, \lceil 2n/3 \rceil}) \sim 2n^3/27 \in \Theta(n^3)$.

Observation 3 *If G is a vertex-transitive graph, then $Mo\,(G) = 0$.*

By the above observation, we have $\mathrm{Mo}\,(K_n) = \mathrm{Mo}\,(C_n) = \mathrm{Mo}\,(K_{n,n}) = 0$. Also $\mathrm{Mo}\,(G) = 0$ for graphs of all Platonic and Archimedean solids, among them for all prisms and antiprisms, and also for the unique fullerene on 60 vertices with full icosahedral symmetry (the buckyball).

Notice, however, that $\mathrm{Mo}\,(G) = 0$ is possible even when G is not vertex-transitive. As an example, take C_{10} and blow-up every second vertex of it into a 3-cycle. More generally, graphs with $\mathrm{Mo}\,(G) = 0$ are exactly the distance-balanced graphs introduced in [14]. A graph G is *distance-balanced* if for every edge uv the number of vertices closer to u than to v is equal to the number of vertices closer to v than to u. Such graphs seem to be well-researched; see, for example, [14] for their basic properties and some open problems. Further, their symmetry properties were investigated in [17], and an interesting connection with Szeged index was explored in [13]. See also [19] for some generalizations. Distance-balanced graphs of even order are also known as *equal opportunity graphs*; see [3] for more details. Hence, the Mostar index measures how far is a graph from being distance-balanced and can be thought of as a quantitative refinement of the distance-non-balancedness of a graph.

We close this section by proving an auxiliary result on a transformation resulting in strictly increased value of $\mathrm{Mo}\,(G)$. The transformation is called the *bridge-to-leaf transformation* and illustrated in Fig. 1.

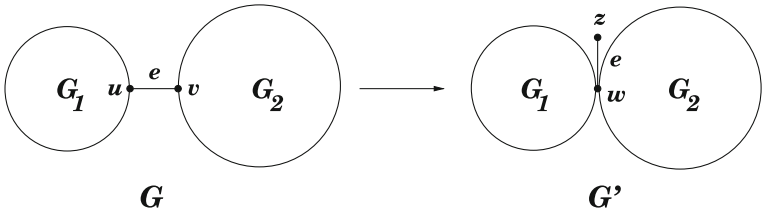


Fig. 1 The bridge-to-leaf transformation

Let G be a connected graph. A set $C \subseteq E(G)$ is called an *edge-cut* if removing the edges of C from G results in a disconnected graph. An edge-cut consisting of one edge is called a *cut-edge* or a *bridge*. A bridge e is *trivial* if one of components of $G - e$ is a single vertex.

Proposition 4 *Let $e = uv$ be a non-trivial bridge in G. Let G' be the graph obtained from G by deleting e from G, identifying u and v into a new vertex w and adding a leaf z connected to w. Let the edge connecting w and z in G' be again denoted by e. Then*

$$Mo\,(G') > Mo\,(G).$$

Proof Observe that after the modification of the graph, for every edge f, distinct from e, the contribution $\phi(f)$ stays unchanged. For edge e, we have that $\phi_G(e) \leq n-3$ as e is a non-leaf in G, and $\phi_{G'}(e) = n-2$ as it is a leaf in G'. Thus, Mo $(G') >$ Mo (G). □

3 Extremal trees and unicyclic graphs

In this section we determine extremal graphs and the corresponding values of Mostar index over trees and unicyclic graphs on a given number of vertices. The case of trees is simpler and we treat it first.

3.1 Trees

It is intuitively clear and it follows easily from the fact that $\phi(e)$ is maximized for edges incident with leaves, that for any tree T_n on n vertices we have

$$\text{Mo}\,(T_n) \leq (n-1)(n-2) = \text{Mo}\,(S_n),$$

with equality if and only if $T_n = S_n$. It is also clear that the next largest value, $(n-2)^2 + n - 4$ is achieved for (and only for) the *broom* $B_{3,n-3}$ obtained by taking a path on 3 vertices and attaching $n-3$ leaves to one of its ends. As expected, the smallest value is achieved for paths.

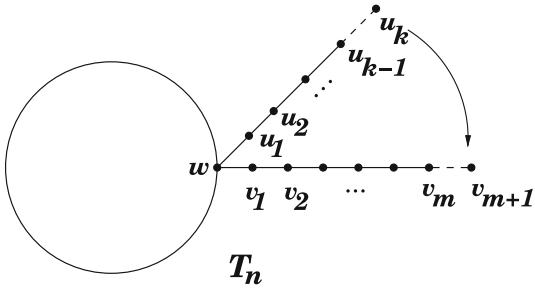


Fig. 2 Mostar index decreasing transformation on trees

Theorem 5 *Let T_n be a tree on n vertices. Then*

$$Mo\,(P_n) = \left\lfloor \frac{(n-1)^2}{2} \right\rfloor \leq Mo\,(T_n) \leq (n-1)(n-2) = Mo\,(S_n),$$

with the left and the right inequality achieved if and only if $T_n = P_n$ and $T_n = S_n$, respectively.

Proof First, observe that formula $\mathrm{Mo}\,(P_n) = 2\left\lfloor \frac{n}{2} \right\rfloor \left\lfloor \frac{n-1}{2} \right\rfloor = \left\lfloor \frac{(n-1)^2}{2} \right\rfloor$ is readily verified by direct computation. The claim of the theorem obviously holds for $n = 2$, so suppose that $n \geq 3$. As we have already settled the upper bound, let us look at the lower one. We have to show that the lower bound is achieved for, and only for, path on n vertices. Let T_n be a tree on $n \geq 3$ vertices that is not a path. Then it has a vertex w of degree at least 3 such that at least two of components of $T_n - w$ are paths. Let their lengths be k and m, where $1 \leq k \leq m$. The situation is shown in Fig. 2. Let T_n' be the tree obtained from T_n by detaching u_k from the end of the shorter path and attaching it as a leaf at v_m, at the end-vertex of the longer path. Now consider the difference $M(T_n) - M(T_n')$. We have

$$\begin{aligned} M(T_n) - M(T_n') &= (n-2k) + (n-2(k-1)) + \cdots + (n-2) + (n-2m) \\ &\quad + \cdots + (n-2) - (n-2(k-1)) - \cdots - (n-2) \\ &\quad - (n-2(m+1)) - (n-2m) - \cdots - (n-2) \\ &= n - 2k - (n-2(m+1)) \\ &= 2m - 2k + 2, \end{aligned}$$

which is always positive. Hence the described transformation strictly decreases the value of Mostar index. Notice that a tree always has a branching vertex w unless it is a path. So applying above operation over and over we must end at P_n as the graph with the smallest Mostar index. □

3.2 Unicyclic graphs

Unicyclic graphs on n vertices consist of a cycle C_k of length $k \geq 3$ and $n-k$ vertices in trees that are "planted" in vertices of the cycle. Let us denote by $S_{n,k}$ the cycle

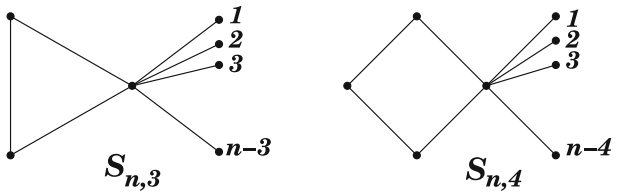


Fig. 3 Extremal unicyclic graphs for Mostar index

of length k with remaining $n-k$ vertices all attached as leaves to the same vertex of the cycle. Graphs $S_{n,3}$ and $S_{n,4}$ are shown in Fig. 3. It will turn out that these two graphs are extremal for the Mostar index. It is not very surprising in view of the fact that large contributions of edges incident to leaves penalize longer cycles, thus promoting unicyclic graphs with the shortest possible cycle C_3 as natural candidates for extremal graphs. However, odd cycles are also penalized by existence of edges whose contribution is zero. The two effects cancel for $n = 8$.

Theorem 6 *Let U_n be a unicyclic graph on $n \geq 3$ vertices. Then*

$$0 = Mo\,(C_n) \leq Mo\,(U_n) \leq Mo\,(S_{n,k}),$$

where $k = 3$ for $3 \leq n \leq 8$ and $k = 4$ for $k \geq 8$. The lower bound is achieved if and only if $U_n = C_n$.

Proof Since C_n is a vertex-transitive graph, $\mathrm{Mo}\,(C_n) = 0$ for all $n \geq 3$. Any unicyclic graph different from C_n must have at least one leaf; since its contribution is equal to $n-2$, it follows $\mathrm{Mo}\,(U_n) \geq n-2$ for all $U_n \neq C_n$. Hence the cycle is the unique unicyclic graph achieving the lower bound of zero.

Let us now look at the upper bound. Let U_n be a unicyclic graph achieving the maximum value of Mostar index. It contains a cycle C_k for some $k \geq 3$. We may assume, due to Proposition 4, that all its vertices not lying on the unique cycle C_k, are leaves. (If there were edges between two non-leaves, each of them would be a bridge, and by performing the bridge-to-leave transformation of Proposition 4 we could obtain a unicyclic graph U_n' with larger value of Mostar index, a contradiction.)

So, we have $m = n-k$ leaves incident to the same number of edges, each of them contributing $n-2$ to the Mostar index. We have to find the arrangement of the leaves that maximizes collective contribution of the edges of C_k.

Let the unique cycle of U_n be $C_k = v_0 v_1 \cdots v_{k-1}$. Let c_i be the number of leaves attached at v_i. Now, we consider two cases with respect to the parity of k and show that all leaves must be adjacent to a same vertex of the cycle.

Suppose first k is even, say $k = 2l$. Notice that for any index i, it holds

$$\phi(v_i v_{i+1}) = |c_{i+1} + c_{i+2} + \cdots + c_{i+l} - c_{i+l+1} - c_{i+l+2} - \cdots - c_i| \leq m.$$

Notice that this contribution attains its maximum value m if all the m leaves are either attached at vertices of the segment $v_{i+1} v_{i+2} \cdots v_{i+l}$ of C or at vertices of the segment

$v_{i+l+1}v_{i+l+2}\cdots v_i$ of C. Now it is easy to see that in order to assure that this holds for every i, it must hold that all m leaves are attached to a same vertex from the cycle.

Now suppose that k is odd, say $k = 2l + 1$. Notice that for any index i, it holds

$$\phi(v_i v_{i+1}) = |c_{i+1} + c_{i+2} + \cdots + c_{i+l} - c_{i+l+2} - c_{i+l+3} - \cdots - c_i| \leq m - c_{i+l+1}.$$

By adding all these inequalities we obtain

$$\sum_i \phi(v_i v_{i+1}) \leq (k-1)m. \tag{1}$$

We obtain equality in (1) if and only if $\phi(v_i v_{i+1}) = m - c_{i+l+1}$ for every i. For a particular i, this is attained, if all the m leaves are either attached at vertices of the segment $v_{i+1}v_{i+2}\cdots v_{i+l}$ of C or at vertices of the segment $v_{i+l+2}v_{i+l+3}\cdots v_i$ of C. Now again it easy to see that in order to assure that this holds for every i, it must hold that all m leaves are attached to a same vertex from the cycle.

By above, U_n is a graph on $n = k + m$ vertices comprised of a cycle of length k with attached m leaves at one particular point of this cycle. If k is even, then

$$\text{Mo}\,(U_n) = m(n-2) + km = m(k+n-2) = n^2 - 2n - k^2 + 2k \leq n^2 - 2n - 8$$

and the upper bound is attained for $k = 4$. And, if k is odd, then

$$\text{Mo}\,(U_n) = m(n-2) + (k-1)m = m(n+k-3) = n^2 - 3n - k^2 + 3k \leq n^2 - 3n,$$

and the upper bound is attained for $k = 3$. Comparing these upper bounds we conclude the statement. Observe that for $n = 8$ the two upper bounds coincide. □

4 Cut method

In this section we show how Mostar index can be efficiently computed for many classes of graphs using a variant of the so-called cut method, introduced back in 1995 by Klavžar, Gutman and Mohar [15]. It was first used to derive closed formulas for Wiener indices of various classes of benzenoid graphs. Indeed, benzenoid graphs are well suited for application of this method since they are partial cubes and their orthogonal cuts coincide with equivalence classes of Djoković–Winkler relation Θ [7,28]. Hence, we will also demonstrate the cut-method on benzenoid graphs. For a very useful survey we refer the reader to [16].

4.1 Benzenoid graphs

Recall that benzenoid graphs can be thought of as parts of an infinite lattice of congruent regular hexagons bounded by a simple closed cycle in the lattice. This definition is somewhat restrictive, but it will suffice for the purpose of demonstration of the cut method. Let us take a benzenoid graph, for example the coronene shown in Fig. 4,

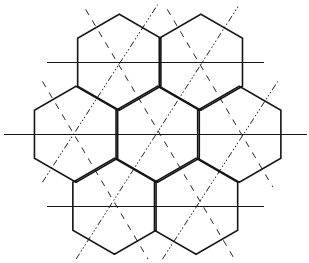


Fig. 4 Coronene and its three families of orthogonal cuts

and draw it in the plane so that some edges are vertical. Obviously, all vertical edges in the same row of hexagons form an edge-cut. Since all of them are intersected at the right angle by a line orthogonal to one of them, we call such a cut *orthogonal cut*. The number of edges in an orthogonal cut is its *size*, and the two components obtained by removing edges of an orthogonal edge-cut are its *shores*. An orthogonal cut is *balanced* if its shores have the same number of vertices. The coronene shown in Fig. 4 has three families of orthogonal cuts, indicated in Fig. 4 by three types of horizontal, ascending, and descending lines intersecting them, respectively.

Following results are immediate consequences of the coincidence of orthogonal cuts with Djoković–Winkler classes in benzenoid graphs.

Proposition 7 *Let e_1 and e_2 be two edges of the same orthogonal cut of a benzenoid graph B. Then their contributions to Mo (B) are equal, i.e., $\phi(e_1) = \phi(e_2)$.*

Proof Recall that two edges $e = xy$ and $f = uv$ of G are in Djoković–Winkler relation if and only if

$$d(x, u) + d(y, v) \neq d(x, v) + d(y, u).$$

It is clear that for every edge e in an orthogonal cut all vertices in one shore of an orthogonal cut (and only those vertices) are closer to the end-vertex of e belonging to the same shore than to the other one. Hence all edges of the same orthogonal cut contribute equally to Mo (B). □

Corollary 8 *Let $F \subset E(B)$ be an orthogonal cut of a benzenoid graph B of size p. If the shores of F have n_1 and n_2 vertices, respectively, then the total contribution of edges from F to Mo (B) is equal to $p|n_1 - n_2|$.*

Corollary 9 *Balanced orthogonal cuts contribute zero to the Mostar index of benzenoid graphs.*

Now we can formulate a general result for Mostar index of benzenoid graphs.

Theorem 10 *Let B be a benzenoid graph on n vertices and let $F_1, \ldots, F_q$ be all its orthogonal cuts. Let p_i denote the size of F_i, and n_{i_1} and n_{i_2} the number of vertices in its shores. Then*

$$Mo\,(B) = \sum_{i=1}^{q} p_i |n_{i_1} - n_{i_2}|.$$

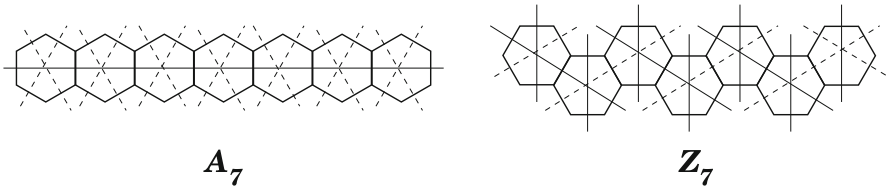


Fig. 5 Polyacene (left) and zig-zag fibonacene (right) of length 7

Since the coronene has six different contributing orthogonal cuts (along with three balanced ones), and since each of them has 3 edges, each edge contributing $19-5 = 14$ to its Mostar index, we obtain $6 \cdot 3 \cdot 14 = 252$ as the value of Mostar index of the coronene.

The cut-method allows us to derive closed formulas for Mostar indices of series of benzenoid graphs of sufficiently high symmetry. We will start, however, with some simpler examples. For the beginning, we compute the Mostar index for two benzenoid chains, a linear polyacene A_q and a zig-zag fibonacene Z_q of the same length q. The chains and their orthogonal cuts are shown in Fig. 5.

Proposition 11 *Let A_q be linear polyacene of length q. Then*

$$Mo\,(A_q) = 32 \left\lfloor \frac{q}{2} \right\rfloor \left\lceil \frac{q}{2} \right\rceil .$$

Proof There are three families of orthogonal cuts. The only member of the horizontal family is balanced and contributes zero. The other two families have equal contributions and it suffices to consider one of them. Let us look at the ascending cuts. There are q of them, each one constituting of 2 edges. Each edge of the leftmost cut contributes $4q + 2 - 3 - 3 = 4(q - 1)$. Each following cut increases by 4 the number of vertices on its left hand side and decreases by 4 the number of vertices on its right-hand side. Hence, the contribution of an edge in kth ascending cut is given by $4(q - 2k + 1)$. Depending on parity of q, the contributions will either hit 0 for an odd q, or skip it by switching from 4 to -4 for an even q, and then become negative with the same trend. Since we are interested only in their absolute value, we may just double the sum of all contributions for $1 \le k \le \lfloor \frac{q}{2} \rfloor$ instead of summing over all $1 \le k \le q$. Hence the total contribution of all ascending cuts is given by

$$\begin{aligned} 2 \cdot 2 \cdot \sum_{k=1}^{\lfloor q/2 \rfloor} 4(q - 2k + 1) &= 16 \left((q+1) \left\lfloor \frac{q}{2} \right\rfloor - 2 \sum_{k=1}^{\lfloor q/2 \rfloor} k \right) \\ &= 16 \left\lfloor \frac{q}{2} \right\rfloor \left(q + 1 - \lfloor \frac{q}{2} \rfloor - 1 \right) = 16 \left\lfloor \frac{q}{2} \right\rfloor \left\lceil \frac{q}{2} \right\rceil . \end{aligned}$$

The claim now follows by doubling the result in order to account also for the contributions of descending cuts. □

Alternatively, we may express Mo (A_q) of linear polyacenes as Mo $(A_q) = 8q^2$ for even q and Mo $(A_q) = 8(q^2 - 1)$ for odd q.

Table 1 The values of Mostar index for the first eight zig-zag fibonacenes and their second differences

q	1	2	3	4	5	6	7	8
Mo (Z_q)	0	32	88	160	256	368	504	656
Δ^2		24	16	24	16	24	16	

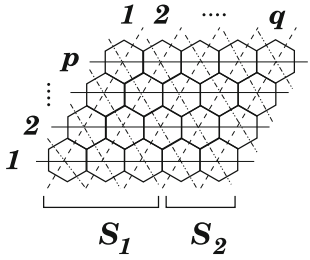


Fig. 6 Benzenoid parallelogram $B_{p,q}$ and its three families of orthogonal cuts

Proposition 12 *Let Z_q be the zig-zag fibonacene of length q. Then*

$$Mo\,(Z_q) = 10q^2 + 4q - 15 - (-1)^q.$$

Proof We could proceed in the same way as in the previous example, but the things here depend on the parity of q in a more complicated way. Instead of analyzing different cases, we notice that both the number of orthogonal cuts and their contributions are linear functions of q. Hence, Mo (Z_q) will be quadratic in q (and in the number of vertices, since it is equal to $4q + 2$). By computing the second differences of the sequence of Mo (Z_q) for $1 \leq n \leq 8$, (shown in Table 1) we observe that they alternate between 24 and 16, depending, as expected, on parity of q. Hence we have two quadratic polynomials giving the values for Mo (Z_q) for even and odd q; by fitting the tabulated values, we obtain Mo $(Z_q) = 10q^2 + 4q - 14$ for odd q and Mo $(Z_q) = 10q^2 + 4q - 16$ for even q. □

As a more complicated example, consider the benzenoid parallelogram $B_{p,q}$ shown in Fig. 6.

Theorem 13

$$\begin{aligned} Mo\,(B_{p,q}) = 4\Bigg[&(p+1)^2\left(\left\lfloor\frac{q}{2}\right\rfloor\left\lceil\frac{q}{2}\right\rceil + \left\lfloor\frac{q-p+1}{2}\right\rfloor\left\lceil\frac{q-p+1}{2}\right\rceil\right) \\ &+(q+1)^2\left\lfloor\frac{p}{2}\right\rfloor\left\lceil\frac{p}{2}\right\rceil\Bigg] \\ &+2(p-1)(p+2)\left[pq+p+q-\binom{p+1}{2}\right]. \end{aligned}$$

Proof Due to symmetry, it suffices to consider the case $p \leq q$. We start by observing that $B_{p,q}$ has $2(pq+p+q)$ vertices arranged into $p+1$ rows. There are three families of cuts. For two of them, the horizontal and the ascending ones, we can apply the same reasoning, while the descending ones require different treatment. We look first at the

horizontal cuts. Each of them consists of $q+1$ vertical edges. Let us look at the horizontal cut containing all vertical edges in kth row. Its total contribution is given by $2(q+1)^2|p+1-2k|$, and the total contribution of all horizontal cuts is obtained by summing over all $1 \le k \le p$ as

$$V = 4(q+1)^2 \left\lfloor \frac{p}{2} \right\rfloor \left\lceil \frac{p}{2} \right\rceil .$$

The total contribution of all ascending cuts is obtained by switching the roles of p and q,

$$U = 4(p+1)^2 \left\lfloor \frac{q}{2} \right\rfloor \left\lceil \frac{q}{2} \right\rceil .$$

Let us now look at the descending cuts. There are $2(p-1)+q-p+1 = p+q-1$ of them. We look at the leftmost $p-1$ cuts first. Let their total contribution be denoted by S_1. The number of edges in them increases by one from 2 in the leftmost one to p in the rightmost one. Hence, the kth cut contains $k+1$ edges. The number of vertices on the left-hand side of the kth cut is equal to $3+5+\cdots+2k+1 = (k+1)^2-1 = k(k+2)$, and contribution of each edge is obtained by subtracting $2k(k+2)$ from the total number of vertices. By summing over all $1 \le q \le p-1$ we obtain the total contribution of the first $p-1$ descending cuts as

$$\begin{aligned} S_1 &= \sum_{k=1}^{p-1} (k+1)\,|2(pq+p+q) - 2k(k+2)| \\ &= (p-1)(p+2)\left[pq+p+q - \binom{p+1}{2} \right]. \end{aligned}$$

Now we look at the $q-p+1$ descending cuts of the same length $p+1$. They are, in fact, the horizontal cuts in $B_{p,q-p+1}$ obtained by discarding the hexagons affected by the cuts contributing to S_1 and their symmetric counterparts in the upper right corner, and rotating the remaining figure counterclockwise by $\pi/3$. Hence, their contribution is given by

$$S_2 = 4(p+1)^2 \left\lfloor \frac{q-p+1}{2} \right\rfloor \left\lceil \frac{q-p+1}{2} \right\rceil .$$

The claim now follows by expressing the total contribution of the descending cuts as $S = 2S_1 + S_2$ and $\mathrm{Mo}\,(B_{p,q}) = V + U + S$. □

Note that for $p = 1$ we recover the formula for the Mostar index of a linear polyacene A_q of length q.

As our final benzenoid example, we consider the circumcoronene series whose first three members are shown in Fig. 7. In general, H_m has $6m^2$ vertices and $6(m-1)$ unbalanced orthogonal cuts besides 3 balanced ones.

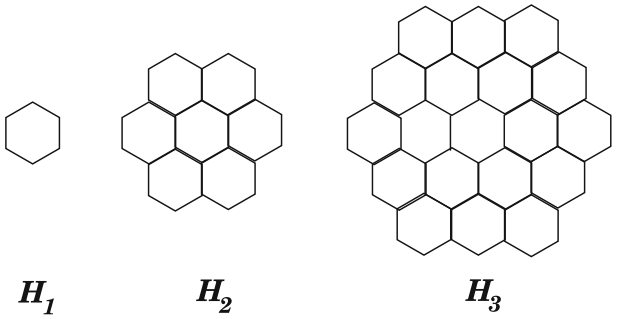


Fig. 7 The first three members in circumcoronene series

Theorem 14

$$Mo\,(H_m) = 9m^2(m-1)(3m+1).$$

Proof Due to symmetry, it suffices to consider $m-1$ horizontal cuts affecting the upper half of H_m. If we denote the uppermost orthogonal cut as the first, then the number of edges in the kth cut is equal to $m+k$, with the contribution of each edge given as $6m^2-4km-2k^2$. The claim now follows by summing all contributions from 1 to $m-1$ and multiplying the result by 6:

$$\mathrm{Mo}\,(H_m) = 6\sum_{k=1}^{m-1}(m+k)(6m^2-4km-2k^2) = 9m^2(m-1)(3m+1).$$

□

The cut-method can be successfully applied also to non-benzenoid graphs whose orthogonal cuts are easy to find. As an example, we compute the Mostar index of a rectangular grid graph $R_{m,n}$ obtained as the Cartesian product of two paths on m and n vertices, respectively.

Theorem 15

$$Mo\,(R_{m,n}) = m^2\left\lfloor\frac{(n-1)^2}{2}\right\rfloor + n^2\left\lfloor\frac{(m-1)^2}{2}\right\rfloor.$$

4.2 Cartesian products

The *Cartesian product* $G\Box H$ of two graphs G and H is defined as the graph on the vertex set that is the Cartesian product of vertex sets of G and H, with the edge set consisting of pairs $(u,v)(u',v')$ where either $u=u'$ and $vv'\in E(H)$, or $v=v'$ and $uu'\in E(G)$. The last result of the previous subsection can be now reformulated as

$$\mathrm{Mo}\,(P_m\Box P_n) = m^2\mathrm{Mo}\,(P_m) + n^2\mathrm{Mo}\,(P_n).$$

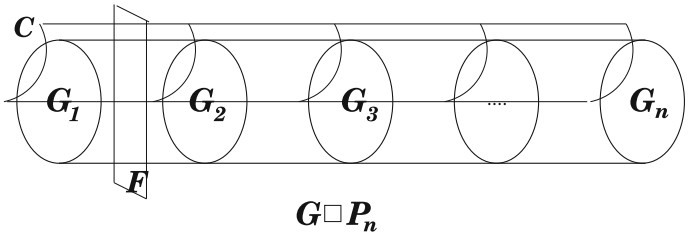


Fig. 8 Computing Mostar index of $G\Box P_n$

This is not accidental; it can be shown that results of this type are valid for Cartesian products of partial cubes. (A *partial cube* is a graph that is an isometric subgraph of a hypercube. See [16] for a more thorough treatment. We just mention here that partial cubes encompass all trees, even cycles, benzenoid graphs, phenylenes, hence many graphs of chemical interest. Also, Cartesian products of partial cubes are again partial cubes.) We illustrate the claim on the case of $G\Box P_n$ shown in Fig. 8.

Proposition 16 *Let G be a partial cube. Then*

$$Mo\,(G\Box P_n) = |V(G)|^2 Mo\,(P_n) + n^2 Mo\,(G).$$

Proof Look at the situation shown in Fig. 8. There are two kinds of orthogonal cuts. One kind, denoted by F in Fig. 8, cuts across the edges between different copies of G. There are $|V(G)|$ edges in one such cut, and their contributions are given in terms of multiples of $|V(G)|$. By summing over all such cuts and factoring out $|V(G)|$ twice, one is left with Mo (P_n), hence the total contribution of all cuts of this type accounts for the first term on the right-hand side of the stated formula.

The other kind of cuts is generated by cuts in G. Let C be one such cut consisting of k edges. Then $C\Box P_n$ is an orthogonal cut in the whole graph. It has nk edges, and its total contribution is obtained by multiplying by n the total contribution of C to Mo (G), since there are n copies of the corresponding shore of G on each of its shores. This gives the total contribution of all such cuts as n^2Mo (G), and the claim follows. □

By completely analogous reasoning one could prove the corresponding result for Cartesian product of general partial cubes. We leave out the details.

Theorem 17 *Let G and H be two partial cubes. Then*

$$Mo\,(G\Box H) = |V(G)|^2 Mo\,(H) + |V(H)|^2 Mo\,(G).$$

5 Open problems and concluding remarks

We have introduced and investigated a new graph-theoretic invariant, the Mostar index, with aim of quantifying the idea of edge peripherality and measuring the graph content of peripheral edges. After introducing some transformations that increase and decrease,

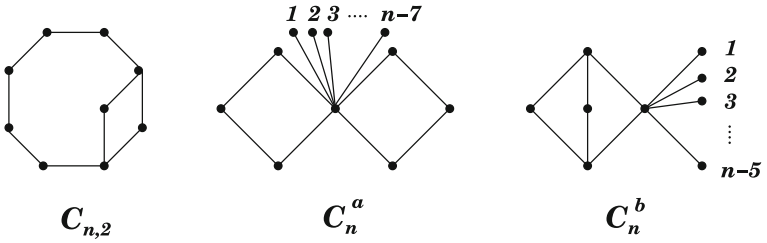


Fig. 9 The conjectured extremal bicyclic graphs

respectively, the value of Mostar index for graphs on the same number of vertices, we have managed to determine the extremal values and graphs for trees and unicyclic graphs. Then we have demonstrated how Mostar index of benzenoids can be efficiently computed by use of a variant of the cut-method applied before to computing various Wiener index-related invariants and showed that the method can be extended to wider classes of graphs. In particular, we have obtained explicit formulas for Cartesian products of partial cubes. There are, however, still many open problems. We start with the case of bicyclic graphs.

5.1 Bicyclic graphs

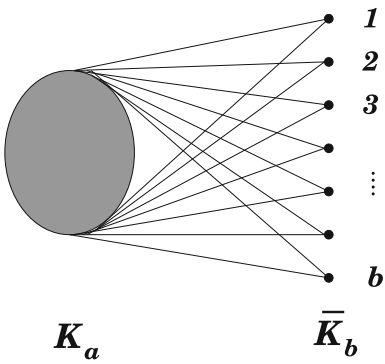
Let $C_{n,2}$ be the graph obtained from C_{n-1} by duplicating just one of it vertices (this new vertex has the same neighbors as it original one). Let C_n^a be the graph obtained by identifying the central vertex of the star S_{n-6} with a vertex of two 4-cycles. Let C_n^b be the graph obtained by identifying the central vertex of the star S_{n-4} with a 2-vertex of a copy of $K_{2,3}$. Note that both graphs C_n^a and C_n^b have n vertices (Fig. 9).

Conjecture 18 *Among all bicyclic graphs on a sufficiently large number of vertices n, $C_{n,2}$ has the smallest and C_n^a and C_n^b have the largest Mostar index.*

It is easy to see that the bicyclic graphs with the smallest possible value of Mostar index cannot contain bridges. Hence, such a graph must be either a splice of two cycles (i.e., a graph obtained by taking two cycles C_a and C_b with $a + b = n + 1$ and identifying one vertex from the first one with one vertex of the second one), or a Θ-graph $\Theta(a, b, c)$ with $a + b + c = n + 2$, where by $\Theta(a, b, c)$ we denote the graph obtained by taking two vertices and connecting them by three paths of lengths a, b, and c that do not have other vertices in common. Numerical evidence for small n seems to rule out the first option and to favor $\Theta(n - 2, 2, 2) = C_{n,2}$ as the optimal choice with $\mathrm{Mo}(C_{n,2}) = n$.

On the other hand, all bridges of a bicyclic graph with the largest value of Mostar index must be incident with leaves. That again means that the two cycles must be either spliced at a single vertex or form a Θ-graph. After some irregularity for small n, numerical evidence suggests both C_n^a and C_n^b as the graphs attaining the largest value of Mostar index with $\mathrm{Mo}(C_n^a) = \mathrm{Mo}(C_n^b) = n^2 - n - 18$. We have not, however, worked out all details.

Fig. 10 Split graph $S_{a,b}$



Besides the extremal bicyclic graphs, there are also other interesting questions. With some of them we close the paper.

5.2 Conjectures and open problems

For the beginning, it would be interesting to investigate how the results of papers concerned with distance-balanced graphs extend to the case $\mathrm{Mo}(G) \neq 0$.

We have already mentioned that $\mathrm{Mo}(K_{\lfloor n/3 \rfloor, \lceil 2n/3 \rceil}) \sim 2n^3/27 \in \Theta(n^3)$. We believe that this is the extremal graph among all bipartite graphs on the same number of vertices.

Conjecture 19 *Among bipartite graphs on n vertices $K_{n/3,2n/3}$ has the maximal Mostar index.*

For general graphs, the extremal graph is most likely the split graph with the same parameters. The *split graph* $S_{m,n}$ is obtained by taking a complete graph K_m on m vertices and n isolated vertices $\overline{K_n}$ and connecting every isolated vertex to all vertices of K_m. A split graph is a join of a complete graph and the complement of another complete graph.

Conjecture 20 *Among all graphs on n vertices the split graph $S_{n/3,2n/3}$ has the maximal Mostar index.*

In order to see that the above two conjectures are at least asymptotically valid, it suffices to consider the case of split graph $S_{a,b}$ shown in Fig. 10. The edges of K_a contribute zero to $\mathrm{Mo}(S_{a,b})$, while each of ab edges between K_a and $\overline{K_b}$ contributes $b-1$. Since $a = n - b$, we have $\mathrm{Mo}(S_{a,b}) = \mathrm{Mo}(b) = b(b-1)(n-b)$. By considering the continuous relaxation and solving the quadratic equation $\frac{d\mathrm{Mo}(b)}{db}$, one readily obtains $b_{max} \sim \frac{2n}{3}$.

We have not investigated how different restrictions (e.g., on the degree, diameter, etc.) affect the extremal graphs for Mostar index. Of particular interest would be to understand behavior of chemically most relevant graphs and trees, those with degree at most four.

Problem 21 *Find chemical graphs and chemical trees on n vertices with largest Mostar index.*

Mostar index of all benzenoid graphs is quadratic in the number of vertices. It is not clear, however, what are the extremal benzenoids. We are inclined to believe that, at least asymptotically, large circumcoronene have the smallest Mostar index among all benzenoids on the same number of vertices. Potential candidates for the largest values could include various fully-leafed and/or snowflake-shaped benzenoids.

Problem 22 *Find extremal benzenoid chains, catacondensed benzenoids and general benzenoid graphs with respect to the Mostar index.*

Our final open problem is concerned with fullerenes. It is well known that the dodecahedron and the buckminsterfullerene are the only two vertex-transitive fullerene graphs. Hence, $\mathrm{Mo}(C_{20}) = \mathrm{Mo}(C_{60} : I_h) = 0$.

Problem 23 *Are there other fullerene graphs G such that* $Mo(G) = 0$*? What are the extremal values and the corresponding graphs?*

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