Mostar index of Cartesian product of graphs and some molecular graphs

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Abstract

On the great success of bond-additive topological indices like Szeged, Padmakar-Ivan, Zagreb, and irregularity measures, yet another index, the Mostar index, has been introduced recently as a peripherality measure in molecular graphs and networks. For a connected graph G, the Mostar index is defined as $M_o(G) = \sum_{e=gh \epsilon E(G)} C(gh)$, where $C(gh) = |n_g(e) - n_h(e)|$ be the contribution of edge uv and $n_g(e)$ denotes the number of vertices of G lying closer to vertex g than to vertex h ($n_h(e)$ define similarly). In this paper, we prove a general form of the results obtained by *Došlić* et al.[4] for compute the Mostar index to the Cartesian product of two simple connected graph. Using this result, we have derived the Cartesian product of paths, cycles, complete bipartite graphs, complete graphs and to some molecular graphs.

Keywords: Molecular graph, Mostar index, Cartesian product.

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1 Introduction

In chemical graph theory, the vertices of a molecular graph G represent the atoms and edges represent the bonds. The shape derived from a chemical compound is often called its molecular graph. Research in mathematical chemistry gives a special attention to capturing the essence of molecular graph and hence, one sometimes wants to associate a unique quantitative value to each chemical compound. One such a characterization in mathematical chemistry is to study the structural invariants of chemical structure, called topological indices or molecular descriptors. An extremely large amount of new topological indices has been introduced and applied for quantitative structure activity relationship(QSAR) and quantitative structure property relationship(QSPR) studies focusing on structure-dependent chemical behavior of molecules. A topological index is a numerical value associated with chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity(e.g., boiling point and melting point). Most of the existing topological indices is mainly based on distances and degree of the given molecular graphs. One of the oldest topological index is Wiener index[24], introduced in 1947, with many chemical applications and mathematical properties and is probably the most studied index from both theoretical and practical points of view (refer[22])belongs to the distance based index, as well as Harary index, total eccentricity index and Balaban index are the few more distance base indices. Zagerb index, Randić index are some of the well studied degree-based indices. Another type of indices called bond-additive indices that measures peripherality of individual bonds (i.e., edges). An edge is peripheral if there are many more vertices closer to one of its end-vertices than to the other one. Sum of the contributions of all edges and produces a global measure of peripherality of a given graph. One such a bond-additive indices has been recently introduced during a small workshop held at the city of Mostar called Mostar index[23]. In the same article, a simple cut method for computing the Mostar index of benzenoid systems was presented. Moreover, extremal trees and unicyclic graphs were studied. Later, the extremal values of the

Mostar index were characterized for bicyclic graphs in reference[1] . Arockiaraj et al.[2] introduce edge-Mostar and total-Mostar indices and obtained these indices for the family of coronoid and carbon nanocone structures. Hayata and Zhoua[8] obtained the n-vertex cacti with the largest Mostar index, and gave a sharp upper bound of the Mostar index for cacti of order n with k cycles. Furthermore, in [6] discussed the Mostar index interms of automorphism of graph and determine for the class of patch fullerence.

Graph operations play an important role in chemical graph theory. Different molecular graphs can be obtained by applying graph operations on some general or particular graphs. Hence it is important to study the various graph operations in order to understand how it is related to the corresponding topological indices of the original graphs. There are several other results regarding various topological indices under different graph operations are available in the literature (see [19, 10]). One of the chemically interseting graph operation is Cartesian product. The linear polynomial chain, nanotube, nanotorus are some of the molecular graphs obtained using Cartesian product. Main aim of this article is to completely settle the exact value of Mostar index to the Cartesian product of any simple connected graphs , which is the general form of the Mostar index to the Cartesian product of partial cubes obtained by *Došlić* et al. in [4]. Using this result we obtained here to the Cartesian product of paths, cycles, complete graph, complete bipartite graph and some molecular structure like cubic corbon and polyacene.

2 Preliminaries

All graphs considered in this paper are simple that is, no loop and multiple edge and connected that is there is a link between any pair of vertices in a graph. A graph G is a pair $G = (V(G), E(G))$ consisting of a finite set $V(G)$ of vertices and $E(G)$ is a set of pairs of elements in $V(G)$. Let $V(G) = \{g_1, g_2, ..., g_n\}$ be the vertex of G and $E(G) = \{g_ig_j |\, g_i, g_j \in V(G)\}$ be an edge set of G. The degree of a vertex

g_i in a graph G is the number of its neighbours and is denoted by $d_G(g_i)$.The distance between the vertices g_j and g_k is the length of the shortest path joining g_j and g_k and is denoted by $d_G(g_j, g_k)$. The complete graph, the path, the cycle the complete equipartite, and the tree on g vertices are denoted by $K_g, P_g, C_g, K_{g,g}$ and T_g respectively.

A vertex $x \in V(G)$ is said to be equidistant from the edge $e = gh$ of G, if $d_G(g, x) = d_G(h, x)$. For an edge $e = (g, h) \in E(G)$, the number of vertices in G whose distance to the vertex g is smaller than the distance to vertex h in G is denoted by $n_G(g, e) = n_g(e)$ and $n_G(h, e) = n_h(e)$ is the number of vertices in G whose distance to the vertex h in G is smaller than to the vertex g; the vertices equidistant form both end point of the edge $e = (g, h)$ are not counted. To expect that interaction of two constitute element will be affected by their distance in the graph.The properties of whole graphs by summing contributions of individual vertcies and edges are called vertex - and bond - additive indices respectively[16, 9].

3 Mostar index of Cartesian Product

For term and concept not define here we refer the reader to any of classical on graph theory. The wiener index of a graph G is defined as the sum of all distance between pair of vertices of G,then now

$$W(G) = \sum_{g,h \in V(G)} d_G(g, h)$$

where $d_G(g, h)$ denotes the usual shortest path distance in G. It was introduced by G Harold Wiener in order to calculate the boiling points of translucent until known it has found various applications chemistry and network theory. For every tree T the wiener index can be computed as the sum of edge contributions more precisely

$$W(T) = \sum_{e=gh \in E(T)} n_g(e) n_h(e)$$

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There are many ways to define meaningful edge contributions, and there are many bond-additive indices, among the best known is, the szeged index introduced by, Gutman in 1994 [7] defined as

$$Sz(G) = \sum_{e=gh \in E(G)} n_g(e) n_h(e)$$

which possesses many interesting applications in chemistry and network theory, and that for any tree T it holds $W(T) = Sz(T)$. Motivated by the success of the Szeged index, some variations were also introduced laterly, one of the interesting descriptor is the Padmakar-Ivan index[14, 12, 15] defined by $PI(G) = \sum_{e=gh \in E(G)} [n_g(e) + n_h(e)]$. Very recently, another intresting bond-additive topological index, named as the Mostar index, has been introduced [1].

Definition 3.1. ***Mostar Index:***
For any connected graph G, the Mostar index of G, denoted as $Mo(G)$, is defined as as the sum of absolute differences between $n_g(e)$ and $n_h(e)$ over all edges $e = gh$ of G.
In short a Mostar index of G is

$$M_o(G) = \sum_{e=gh \epsilon E(G)} |n_g(e) - n_h(e)|$$

The absolute difference $|n_g(e) - n_h(e)|$ will be called the contribution of edge $e = gh$ and denoted by $C(gh)$, so as the Mostar index equivalently expressed as a

$$M_o(G) = \sum_{e=gh \in E(G)} C(gh)$$

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Graph operation play an important role in studied of graph decomposition into isomorphic sub graph.It is well known that many graphs arise from simple graphs

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via various graph operation and one can study the properties of smaller graphs and deriving with it some information about larger graphs, Hence it is important to understand how certain invariant of such product graphs are related to corresponding invariant of the original graphs. The Cartesian product is an important method to construct a bigger graph and plays an important role in the design and analysis of networks [25]. Throughout the paper we will use the following notation;
For a connected graph $G, H,$ let the vertex set of G is $V(G) = \{g_1, g_2, g_3........g_n\}$ and the vertex set of H is $V(H) = \{h_1, h_2, h_3........h_m\}$.

Definition 3.2. ***Cartesian Product:***
Cartesian product of G and H is a graph, denoted by $G\square H$,with the vertex set $V(G\square H) = \{(g_i, h_r)|g_i \in V(G), h_r \in V(H)\}$ and any two vertices (g_i, h_r) (g_j, h_s) are adjacent in $G\square H$ if and only if $g_i = g_j$ and $h_r h_s \in E(H)$ or $g_i g_j \in E(G)$ and $h_r = h_{s.}$

For our convenience, we partition the edge set of $G\square H$ into two set
$E_1 = \{(g_j, h_l), (g_j, h_m)|g_j \in V(G), h_l h_m) \in E(H)\}$
and $E_2 = \{(g_j, h_l)(g_k, h_l)|g_j g_k \in E(G), h_l \in V(H)\}$, that is E_1 denoted the edges of the copies of H corresponding to the vertices of G and E_2 denotes the edges of the copies of G to the vertices of H .
Clearly the above definition yield the lemma stated below.

Lemma 3.1. *Let G and H be graphs. Then we have:*
(i) $|V(G\square H)| = |V(G)||V(H)|, |E(G\square H) = |E(G)||V(H)| + |E(H)||V(G)|$
(ii)If (g_i, h_l) *and* (g_j, h_m) *are vertices of* $G\square H,$ *then* $d_{G\square H}[(g_i, h_l), (g_j, h_m)] = d_G(g_i, g_j) + d_H(h_l, h_m)$
(iii) $d_{G\square H}[g_i, h_l)] = d_G(g_i) + d_H(h_l)$
(iv) $G\square H$ *cis connected if and only if* G *and* H *are connected.*
(v) The Cartesian product is commutative and associative.
For an edge $e = g_i g_j \in E(G)$ *, let* $T_G(e; g_i)$ *be the set of vertices closer to* g_i *than* g_j *and* $T_G(e; g_j)$ *be the set of vertices closer to* g_j *than* g_i *. That is* $T_G(e; g_i) = [g_l \in$

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$V(G)|d_G(g_i,g_l) < d_G(g_j,g_l)]$ and let $T_G(e;g_j) = [g_l \in V(H)|d_G(g_j,g_l) < d_G(g_i,g_l)]$ respectively[11, 21].

As a consequence of the main theorem obtained in [11], we have observe the following as a lemma which is applied in our main result:

Lemma 3.2. *Let G and H be graphs. Then for any edge e in the edge partition E_1 , E_2 of $G\Box H$ as defined above, we have*
$n_{G\Box H}((g_r,h_i),e) = |V(G)|n_H(h_i,e)$,
$n_{G\Box H}((g_r,h_k),e) = |V(G)|n_H(h_k,e)$ *and*
$n_{G\Box H}((g_i,h_l),e) = |V(H)|n_G(g_i,e)$,
$n_{G\Box H}((g_k,h_l),e) = |V(H)|n_G(g_k,e)$ *respectively.*

For convenience we introduce the following notation. Let $|V(G)| = V_{|G|}$ and $|V(H)| = V_{|H|}$ denote the number of vertices in G and H respectively. To the continuation of the above discussion, now we move to the main results of this section by obtaining the Mostar index to the Cartesian product of two graphs.

Theorem 3.1. *Let G and H be two connected graphs. Then we have $M_o(G\Box H) = V_{|H|}^2 M_o(G) + V_{|G|}^2 M_o(H)$ where $V_{|G|}, V_{|H|}$ be the order of vertex set of the graph G,H respectively.*

Proof:
Let $|V(G)| = V_{|G|}$ and $|V(H)| = V_{|H|}$ be the number of vertices in G and H respectively. Assume that the edge set of $G\Box H$ is partitioned into E_1 and E_2 as defined early. Then by the definition of Mostar index of graph $G\Box H$, we have

$$M_o(G\Box H) = \sum_{xy=e'=E(G\Box H)} C(gh)$$

$$= \sum_{xy=e'=E(G\Box H)} |n_{G\Box H}(x,e') - n_{G\Box H}(y,e')|$$

By applying the above lemma [3.1] and [3.2], we have

$$M_o(G\Box H) = \sum_{e'=(g_r,h_i)(g_r,h_k)\epsilon E_1} |n_{G\Box H}((g_r,h_i),e') - n_{G\Box H}((g_r,h_k),e')|$$

$$+ \sum_{e'=(g_i,h_l)(g_k,h_l)\epsilon E_2} |n_{G\Box H}[(g_i,h_l),e'] - n_{G\Box H}((g_k,h_l),e')|$$
$$= \sum_{e=(h_i,h_k)\epsilon E_1} \left|V_{|G|}n_H(h_i,e) - V_{|G|}n_H(h_k,e)\right|$$
$$+ \sum_{e=(g_i,g_k)\epsilon E_2} \left|V_{|H|}n_G(g_i,e) - V_{|H|}n_G(g_k,e)\right|$$
$$= V_{|G|} \sum_{e=(h_i,h_k)=E_1} |n_H(h_i,e) - n_H(h_k e)| + V_{|H|} \sum_{e=(g_i,g_k)=E_2} |n_G(g_i,e) - n_G(g_k,e)|$$
$$= V_{|G|}V_{|G|}M_o(H) + V_{|H|}V_{|H|}M_o(G)$$
$$= V_{|G|}^2 M_o(H) + V_{|H|}^2 M_o(G)$$

This completes the proof.

It is easy to observe from the refrence[23], the Mostar index of path is

$$M_o(P_g) = \begin{cases} \dfrac{(g-1)^2}{2} & : \text{ if g is odd,} \\ \dfrac{g(g-2)}{2} & : \text{ if g is even,} \end{cases}$$

The proof of the following corollaries are directly follows from the main Theorem 3.1.

Corollary 3.1. *Let P_g and P_h be a path on g and h vertices respectively, then*

$$M_o(P_g \Box P_h) = \begin{cases} \dfrac{gh}{2}(2gh - g - h) & : \textit{ if g and h is even,} \\ \dfrac{g^2+h^2}{2} + gh(gh+g+h) & : \textit{ if g and h is odd} \\ \dfrac{(h(h-g^2))}{2} + gh^2(g-1 & : \textit{ if g is odd,h is even} \end{cases}$$

A graph G is said to be a vertex transitive if for every pair $g_i, g_j \in V$ there exists an automorphism f that maps g_i to g_j.

Corollary 3.2. *[13] For a graph G, H and if H is a vertex transitive, then $M_o(G \Box H) = V_{|H|}^2 M_o(G)$.*

Proof: Given that H is a vertex transitive graph then its Mostar index $M_o(H) = 0$ [23]. So by the Theorem 3.1., we have

$$M_o(G \Box H) = V_{|H|}^2 M_o(G)$$

From the above Corollary 3.2., if G is also vertex transitive, then $M_o(G \Box H) = 0$. Since some of the standard graphs like the cycle, the complete graph, the complete

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equibipartite graph and some molecular graph like platonic, the Archimedean solids, prisms and antiprisms and also for the unique fullerene on 60 vertices with full icosahedral symmetry (the buckyball) are vertex transitive, we hav the following examples:

1. $M_o(P_g \Box K_h) = V^2_{|K_h|} M_o(P_g)$
2. $M_o(P_g \Box C_h) = V^2_{|C_h|} M_o(P_g)$
3. $M_o(P_g \Box K_{h,h}) = V^2_{|K_{h,h}|} M_o(P_g)$
4.If a graph H is Platonic, Archimedean solids, all prisms and anti prisms, then we have $M_o(G \Box H) = V^2_{|H|} M_o(G)$
5.If H is a unique fullerene on 60 vertices with full icosahedral symmetry (the buckyballs) $M_o(G \Box H) = V^2_{|H|} M_o(G)$.

Corollary 3.3. *For any graph G and for any tree T on n vertices, then* $M_o(G \Box T) \le n^2 M_o(G) + V^2_{|G|}(n-1)(n-2)$

Proof: By direct calculation, using the main Theorem 3.1. we have
$M_o(G \Box T) = n^2 M_o(G) + V^2_{|G|} M_o(T)$
$\le n^2 M_O(G) + V^2_{|G|}(n-1)(n-2)$, since $M_o(T) \le (n-1)(n-2)$ [23]
with equality is hold iff $T = S_{1,n-1}$ star on n vertices.
A broom $B_{k,n-k}$ is a tree obtained by taking a path on k vertices and attaching $n-k$ leaves to one of its ends.

Corollary 3.4. *For any graph G and if $H = B_{3,n-3}$ is Broom,then* $M_o(G \Box B_{3,n-3}) = n^2 M_o(G) + V^2_{|G|}\big((n-2)^2 + (n-4)\big)$.

Proof: By directly calculation, using the main Theorem 3.1. we have
$M_o(G \Box B_{3,n-3}) = n^2 M_o(G) + V^2_{|G|} M_o(B_{3,n-3})$
$= n^2 M_o(G) + V^2_{|G|}\big((n-2)^2 + (n-4)\big)$, since $M_o(B_{3,n-3}) = \big((n-2)^2 + (n-4)\big)$[23].

4 Mostar index of some molecular graphs

In this section, we consider some of the molecular structures and obtain its Mostar index. One of the many chemical compounds that are useful and necessary for the survival of living organisms are carbon, oxygen, hydrogen and nitrogen. These are helpful for the production of cells in the living organisms. Carbon is an essential element for the formation of proteins, carbohydrates and nucleic acids. The carbon atoms can bond together in various ways, called allotropes of carbon. The well known forms are graphite and diamond. Recently, many new forms have been discovered including nanotubes, buckminster fullerene and sheets, crystal cubic structure, etc. The structure of crystal cubic carbon consist of cubes and some of the its topological indices were discussed in [3, 9]. The molecular graph of crystal cubic carbon $CCC(n)$ at various level is depicted in Fig. 2(a).To obtain the Mostar index of crystal cubic carbon $CCC(n)$, we have consider the following edge partition of all the edges of $CCC(n)$. Let Q_1 be the set of 12 edges in the first level, Q_j be the set of $96(7)^{j-2}$ edges in all new cubes at j-th level and R_j be the set of $8(7)^{j-2}$ edges that connects the cubes of j-th level to cubes of $(j-1)$-th level. As a consequence of the results obtained in [3], we have observe the following as a lemma which is applied in our main result:

Lemma 4.1. *[9] Let the graph $G \cong CCC(n)$ be a crystal cubic carbon on n-vertices. Then for any edge $e = uv$ in Q_1, Q_j and R_j of $CCC(n)$, we have*
$n_u(e) = \frac{16}{21}7^n - \frac{4}{3}$, $n_v(e) = \frac{16}{21}7^n - \frac{4}{3}$
$n_u(e) = \frac{16}{21}7^{n-j+1} - \frac{4}{3}$, $n_v(e) = \frac{32}{21}7^n - \frac{4}{3} - \frac{16}{3}7^{n-j}$ *and*
$n_u(e) = 8^{n-j+1}$, $n_v(e) = \frac{32}{21}7^n - \frac{8}{3} - 8^{n-j+1}$ *respectively.*

Theorem 4.1. *Let the graph G be the crystal cubic carbon $CCC(n)$ with n vertices. Then the Mostar index of crystal cubic carbon is*

$$M_o(CCC(n)) = \frac{512\big(7^n\big)\big(7^n - 6n - 1\big)}{147} + 64\left(\frac{\big(4(7^{n-1}) - 1\big)\big(7^{n-1} - 1\big)}{18} - 2\Big(8^{(n-1)} - 7^{(n-1)}\Big)\right).$$

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Proof:

Since by the definition of Mostar index of graph and by the edge partition of $CCC(n)$ as discussed above we have,

$M_o(CCC(n)) = \sum_{e=uv\epsilon E(CCC(n))} |n_u(e) - n_v(e)|$

$= \sum_{e=uv\epsilon E(Q_1)} |n_u(e) - n_v(e)| + \sum_{e=uv\epsilon E(Q_j)} |n_u(e) - n_v(e)| + \sum_{e=uv\epsilon E(R_j)} |n_u(e) - n_v(e)|$

$= M_o(Q_1) + M_o(Q_j) + M_o(R_j)$ ....(1)

Now to obtained each summation seprately, by using the Lemma 4.1., we have the following $M_o(Q_1) = 12\left|\left(\frac{16}{21}7^n - \frac{4}{3}\right) - \left(\frac{16}{21}7^n - \frac{4}{3}\right)\right| = 0$ ....(2)

$$M_o(Q_j) = \sum_{j=2}^{n} 96(7)^{j-2}\left|\left(\frac{16}{21}7^{n-j+1} - \frac{4}{3}\right) - \left(\frac{32}{21}7^n - \frac{4}{3} - \frac{16}{3}7^{n-j}\right)\right|$$

$= 512\sum_{j=2}^{g} 7^{g+j-2}\left|\frac{7-7^j}{7^{j+1}}\right|$

$= 512\sum_{j=2}^{n}(7)^{n-3}\left|2\left(7^{1-j}-1\right)\right|$

$= 1024\sum_{j=2}^{n}(7)^{n-3}\left|7-7^j\right|$

$= 1024\sum_{j=2}^{n}(7)^{n-2}\left(7^{j-1}-1\right)$

$= 1024(7)^{n-2}\left(\frac{7\left(7^{n-1}-1\right)}{6} - (n-1)\right)$

$= \frac{512\left(7^n\right)\left(7^n - 6n - 1\right)}{147}$ ....(3)

and $M_o(R_j) = \sum_{j=2}^{n} 8(7)^{j-2}\left|8^{n-j+1} - \left(\frac{32}{21}7^n - \frac{8}{3} - 8^{n-j+1}\right)\right|$

$= 64\sum_{j=2}^{n}(7)^{j-2}\left|2(8)^{n-j} - \frac{4}{21}7^n + \frac{1}{3}\right|$ ....(4)

Since $\frac{4}{21}7^n > 2(8)^{n-j} + \frac{1}{3}$, we have

$= 64\sum_{j=2}^{n}(7)^{j-2}\left(\frac{4}{21}7^n - \left(2(8)^{n-j} + \frac{1}{3}\right)\right)$

$= 64\sum_{j=2}^{n}\left(\left(\frac{4(7^{n-1})-1}{3}\right)(7)^{j-2} - 2(8)^{(n-j)}(7)^{(j-2)}\right)$

$= 64\left(\left(\frac{4(7^{n-1})-1}{3}\right)\sum_{j=2}^{n}(7)^{j-2} - 2\frac{8^n}{49}\sum_{j=2}^{n}\left(\frac{7}{8}\right)^j\right)$

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$$= 64\left(\frac{\left(4(7^{n-1})-1\right)\left(7^{n-1}-1\right)}{18} - 2(8)^{(n-1)}\left(1-\left(\frac{7}{8}\right)^{n-1}\right)\right)$$
$$= 64\left(\frac{\left(4(7^{n-1})-1\right)\left(7^{n-1}-1\right)}{18} - 2\left(8^{(n-1)}-7^{(n-1)}\right)\right)$$

Hence substitute the equations (2),(3) and (4) in (1), we have

$$M_o(CCC(n)) = 0 + \frac{512\left(7^{n}\right)\left(7^{n}-6n-1\right)}{147} + 64\left(\frac{\left(4(7^{n-1})-1\right)\left(7^{n-1}-1\right)}{18} - 2\left(8^{(n-1)}-7^{(n-1)}\right)\right).$$

Theorem 4.2. *Let the graph G be the Polycyclic Aromatic Hydrocarbons PAH_k with $k \geq 1$. Then the Mostar index of Polycyclic Aromatic Hydrocarbons PAH_k is* $M_o(PAH_k) = 6k(3k-1)\Big[k(3k+2) - \Big(\frac{k(k-1)(2k-1)}{6} + k(k-1)\Big)\Big]$.

Proof:

Consider the general form of the molecular graph Polycyclic Aromatic Hydrocarbons PAH_k ($k \geq 1$) with $6k^2+6k$ vertices and $9k^2+3k$ edges. Using the result obtained in [5, 17] by the method of orthogonal cut C_i for every $i = 0, 1, 2 \cdots k$, $n_v = i^2 + 2(k+1)i + k$ and $n_u = 6k^2 + 5k - i^2 - 2(k+1)i$. From the definition of Mostar index we have the following

$$M_o(PAH_k) = \sum_{e=uv\epsilon E(PAH_k)} |n_u(e) - n_v(e)|.$$
$$=6k\sum_{e\epsilon C_k} |n_u(e) - n_v(e)| + 6\sum_{e\epsilon C_i, i=0}^{k-1} (k+i)\,|n_u(e) - n_v(e)|$$
$$= 0 + 6\sum_{i=0}^{k-1}(k+i)\left|(i^2+2(k+1)i+k) - (6k^2+5k-i^2-2(k+1)i)\right|$$
$$= 6\sum_{i=0}^{k-1}2(k+i)\left|i^2+2(k+1)i-2k-3k^2\right|$$
$$= 6\left[2\left(k^2+\tfrac{k(k-1)}{2}\right)(3k^2+2k) - 2\left(k^2+\tfrac{k(k-1)}{2}\right)\left(\frac{(k-1)k(2k-1)}{6} + k(k-1)\right)\right]$$
$$= 6k(3k-1)\Big[k(3k+2) - \Big(\frac{k(k-1)(2k-1)}{6} + k(k-1)\Big)\Big].$$

Example 4.1 *The Vertex-Mostar index of circumcoronene* $H_3, M_o(H_3) = 1620$ *[19]*

since there exists orthogonal cuts and implies that $n_{g_1} = 7, n_{h_1} = 47, n_{g_2} = 16, n_{g_2} = 38, n_{g_3} = 27, n_{h_3} = 27$

The number of repetition of first second and third orthogonal cuts are equal to 6, 6 and 3 respectively, [18] Hence, $M_o(H_3) = \sum_{e \epsilon E(H_3)} |n_g(e|H_3) - n_h(e|H_3)|$

$= (6 * 4\,|7 - 47|) + (6 * 5\,|16 - 38|) + (3 * 6\,|27 - 27|)$

$= (24 * 40) + (30 * 22) + 0$

$= 960 + 660$

$M_0(H_3) = 1620$

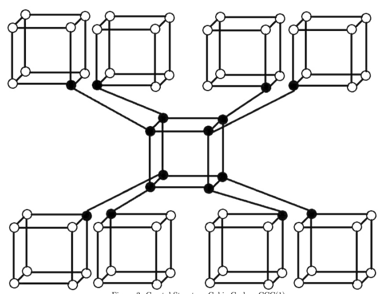
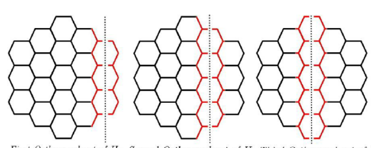


Figure 3. Crystal Structure Cubic Carbon CCC(1)



First Orthogonal cut of H_3 *Second Orthogonal cut of* H_3 *Third Orthogonal cut of* H_3

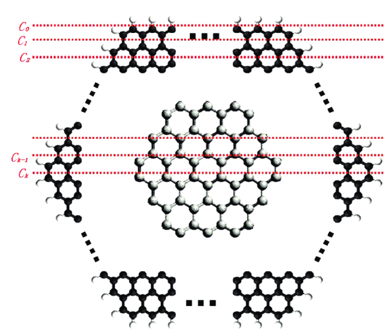


Figure 4: All Orthogonal cuts of PAH_k

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