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Circumcoronene Nanostructures with Cavity and its Novel Molecular Descriptors

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Abstract:-A topological descriptor is a mathematical value related with chemical structure for relationship of chemical structure with a variety of physical properties, chemical reactivity otherwise biological activity. Quantitative structure activity and structure property relation of chemical structure need expressions intended for the topological property of these structures. In this paper, we present the exact expression for various molecular bond additive descriptors for circumcoronene and hexa-peri-hexabenzocoronene Nanostructures with cavity.

Keywords*: Circumcoronene Nanostructures, hexa-peri-hexabenzocoronene, chemical structure.*

1. Introduction

Chemical graph theory is a field within mathematical chemistry that utilises graph theory for the purpose of mathematically modelling chemical events $[1-4]$. This theory had an important influence on the growth of the chemical and molecular sciences. Chemical graph theory is a crucial component in the study of QSAR/QSPR, as it aids in the modelling of organic chemical networks. This involves transforming the original chemical compounds into hydrogen-exhausted graphs, where the vertices represent points and the bonds by lines. The concept of chemical graph hypothesis involves the use of graph theory to the numerical modelling of chemical events, specifically focusing on the topological partitioning within numerical chemistry. The proponents of the theory maintain the characteristic of a chemical graph, which refers to a graph that provides valuable insights into the phenomena of a material through a hypothetical illustration of its particles. Molecules and molecular compounds are commonly represented using molecular graphs $[5-14]$. Let $G = (V(G), E(G))$ be the molecular graph. The cardinality of these sets reflects the respective number of vertices and edges. An edge with the ending vertices u and v in $E(G)$ is denoted by $e = uv$. If there is an edge between them, two vertices, $u$and v, are said to be adjacent.

2. Bond Additive Descriptors

Many molecular descriptors are defined based on its bond additiveness. Firstly, we categorizethe edges of a molecular graph and we proceed with the descriptor Des calculation based on the general expression as given in [15]

$$Des(G) = \sum_{uv \in E(G)} f(d_G(u), d_G(v))$$

here the set $E(G)$ is the collection of edges and f is a function that maps a real value to an ordered pair which defines an edge. If the ordered pair does not contribute an edge, then we count null for that case. Since there are several ways of determining f, it is clear that this definition is fairly broad.

Randic type lordeg index:

$$RLI(G) = \sum_{\{u,v\}\subset V(G)} \ln(d_u)\ln(d_v)$$

Sum lordeg index:

$$SLI(G) = \sum_{\{u,v\}\subset V(G)} \sqrt{\ln(d_u)} + \sqrt{\ln(d_v)}$$

lnverse sum lordeg index:

$$ISLI(G) = \sum_{\{u,v\}\subset V(G)} \frac{1}{\sqrt{\ln(d_u)} + \sqrt{\ln(d_v)}}$$

lnverse sum indeg index:

$$ISI(G) = \sum_{\{u,v\}\subset V(G)} \frac{d_u d_v}{d_u + d_v}$$

Misbalance lordeg index:

$$MLI(G) = \sum_{\{u,v\}\subset V(G)} |\ln(d_u) - \ln(d_v)|$$

Misbalance losdeg index:

$$MLSI(G) = \sum_{\{u,v\}\subset V(G)} |\ln^2(d_u) - \ln^2(d_v)|$$

Misbalance indeg index:

$$MII(G) = \sum_{\{u,v\}\subset V(G)} \left|\frac{1}{d_u} - \frac{1}{d_v}\right|$$

Misbalance irdeg index:

$$MIRI(G) = \sum_{\{u,v\}\subset V(G)} \left|\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}}\right|$$

Misbalance rodeg index:

$$MRI(G) = \sum_{\{u,v\}\subset V(G)} |\sqrt{d_u} - \sqrt{d_v}|$$

Misbalance deg index:

$$MDI(G) = \sum_{\{u,v\}\subset V(G)} |d_u - d_v|$$

Misbalance hadeg index:

$$MHI(G) = \sum_{\{u,v\}\subset V(G)} \left|\left(\frac{1}{2}\right)^{d_u} - \left(\frac{1}{2}\right)^{d_v}\right|$$

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Min-max rodeg index:

$$MMRI(G) = \sum_{\{u,v\}\subset V(G)} \sqrt{\frac{\min(d_u, d_v)}{\max(d_u, d_v)}}$$

Max-min rodeg index:

$$MMRDI(G) = \sum_{\{u,v\}\subset V(G)} \sqrt{\frac{\max(d_u, d_v)}{\min(d_u, d_v)}}$$

Max-min deg index:

$$MMDI(G) = \sum_{\{u,v\}\subset V(G)} \frac{\max(d_u, d_v)}{\min(d_u, d_v)}$$

Max-min sdeg index:

$$MMSDI(G) = \sum_{\{u,v\}\subset V(G)} \left(\frac{\max(d_u, d_v)}{\min(d_u, d_v)}\right)^2$$

Symmetric division deg index:

$$SDDI(G) = \sum_{\{u,v\}\subset V(G)} \frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)}$$

3. CircumcoroneneSeries with Cavity $CC(n,r)$

This section finds bond additive molecular descriptors of $CC(n,r)$. There are $6n^2 - 12r + 6$, vertices and $9n^2 - 9r^2 - 3n - 3r$ edges of $CC(n,r)$ respectively, see in Figure 1. The bonds of $CC(n,r)$ are classified into three types as shown in Table 1.

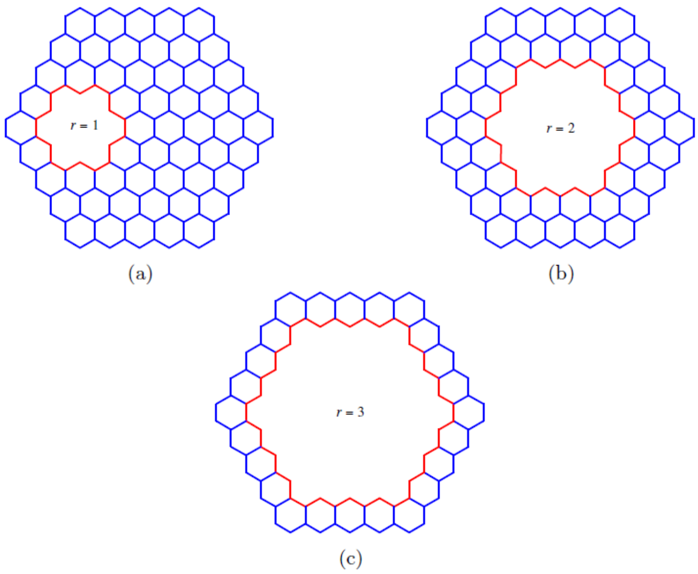

Figure 1: (a) $CC(5,1)$; (b) $CC(5,2)$; (b) $CC(5,3)$

Table 1: The edge partition of circumcoronene series with cavity $CC(n,r)$

(d_u, d_v)	Number of edges in $CC(n,r)$

(2, 2)	6
(2,3)	$12(n + r - 1)$
(3,3)	$9n^2 - 9r^2 - 15n - 15r + 6$

Theorem 1. Let G be a $CC(n,r)$, then

(i) $RLI(CC(n,r)) = 10.8625n^2 - 10.8625r^2 - 8.9662n - 8.9662r + 0.9864.$

(ii) $SLI(CC(n,r)) = 18.8666n^2 - 18.8666r^2 - 8.876n - 8.876r + 0.0001.$

(iii) $ISLI(CC(n,r)) = 4.2933n^2 - 4.2933r^2 - 0.7749n - 0.7749r + 0.085.$

(iv) $ISI(CC(n,r)) = 13.5n^2 - 13.5r^2 - 8.1n - 8.1r - 0.6.$

(v) $MLI(CC(n,r)) = 4.8656n + 4.8656r - 4.8656.$

(vi) $MLSI(CC(n,r)) = 8.718n + 8.718r - 8.718.$

(vii) $MII(CC(n,r)) = 2n + 2r - 2.$

$(viii)$ $MIRI(CC(n,r)) = 1.5571n + 1.5571r - 1.5571.$

(ix) $MRI(CC(n,r)) = 3.814n + 3.814r - 3.814.$

(x) $MDI(CC(n,r)) = 12n + 12r - 12.$

(xi) $MHI(CC(n,r)) = 1.5n + 1.5r - 1.5.$

(xii) $MMRI(CC(n,r)) = 9n^2 - 9r^2 - 5.202n - 5.202r + 2.202.$

$(xiii)$ $MMRDI(CC(n,r)) = 9n^2 - 9r^2 - 0.3031n - 0.3031r - 2.6969.$

(xiv) $MMDI(CC(n,r)) = 9n^2 - 9r^2 + 3n + 3r - 6.$

(xv) $MMSDI(CC(n,r)) = 9n^2 - 9r^2 + 12n + 12r - 15.$

(xvi) $SDDI(CC(n,r)) = 18n^2 - 18r^2 - 4n - 4r - 2.$

Proof.

$$RLI\big(CC(n,r)\big) = \sum_{uv\in E(G)} \ln d_G(u) \ln d_G(v)$$

$$= (\ln 2 \times \ln 2)(6) + (\ln 2 \times \ln 3)(12(n + r - 1)) + (\ln 3 \times \ln 3)(9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 10.8625n^2 - 10.8625r^2 - 8.9662n - 8.9662r + 0.9864.$$

$$SLI\big(CC(n,r)\big) = \sum_{uv\in E(G)} \sqrt{\ln (d_u)} + \sqrt{\ln (d_v)}$$

$$= \left[\sqrt{\ln 2 \times \ln 2}\right](6) + \left[\sqrt{\ln 2 \times \ln 3}\right](12(n + r - 1)) + \left[\sqrt{\ln 3 \times \ln 3}\right](9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 18.8666n^2 - 18.8666r^2 - 8.876n - 8.876r + 0.0001.$$

$$ISLI\big(CC(n,r)\big) = \sum_{uv\in E(G)} \frac{1}{\sqrt{\ln (d_u)} + \sqrt{\ln (d_v)}}$$

$$= \left[\frac{1}{\sqrt{\ln(2)} + \sqrt{\ln(2)}}\right](6) + \left[\frac{1}{\sqrt{\ln(2)} + \sqrt{\ln(3)}}\right](12(n + r - 1)) + \left[\frac{1}{\sqrt{\ln(2)} + \sqrt{\ln(3)}}\right](9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 4.2933n^2 - 4.2933r^2 - 0.7749n - 0.7749r + 0.085.$$

$$ISI(CC(n,r)) = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u + d_v}$$

$$= \left[\frac{2\times 2}{2+2}\right](6) + \left[\frac{2\times 3}{2+3}\right](12(n + r - 1)) + \left[\frac{3\times 3}{3+3}\right](9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 13.5n^2 - 13.5r^2 - 8.1n - 8.1r - 0.6.$$

$$MLI(CC(n,r)) = \sum_{uv\in E(G)} |\ln(d_u) - \ln(d_v)|$$

$$= |\ln(2) - \ln(2)|(6) + |\ln(2) - \ln(3)|(12(n + r - 1)) + |\ln(3) - \ln(3)|(9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 4.8656n + 4.8656r - 4.8656.$$

$$MLSI(CC(n,r)) = \sum_{uv\in E(G)} |\ln^2(d_u) - \ln^2(d_v)|$$

$$= |\ln^2(2) - \ln^2(2)|(6) + |\ln^2(2) - \ln^2(3)|(12(n + r - 1)) + |\ln^2(3) - \ln^2(3)|(9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 8.718n + 8.718r - 8.718.$$

$$MII(CC(n,r)) = \sum_{uv\in E(G)} \left|\frac{1}{d_u} - \frac{1}{d_v}\right|$$

$$= \left|\frac{1}{2} - \frac{1}{2}\right|(6) + \left|\frac{1}{2} - \frac{1}{3}\right|(12(n + r - 1)) + \left|\frac{1}{3} - \frac{1}{3}\right|(9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 2n + 2r - 2.$$

$$MIRI(CC(n,r)) = \sum_{uv\in E(G)} \left|\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}}\right|$$

$$= \left|\tfrac{1}{\sqrt{2}} - \tfrac{1}{\sqrt{2}}\right|(6) + \left|\tfrac{1}{\sqrt{2}} - \tfrac{1}{\sqrt{3}}\right|(12(n + r - 1)) + \left|\tfrac{1}{\sqrt{2}} - \tfrac{1}{\sqrt{3}}\right|(9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 1.5571n + 1.5571r - 1.5571.$$

$$MRI(CC(n,r)) = \sum_{uv\in E(G)} |\sqrt{d_u} - \sqrt{d_v}|$$

$$= |\sqrt{2} - \sqrt{2}|(6) + |\sqrt{2} - \sqrt{3}|(12(n + r - 1)) + |\sqrt{3} - \sqrt{3}|(9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 3.814n + 3.814r - 3.814.$$

$$MDI(CC(n,r)) = \sum_{uv\in E(G)} |d_u - d_v|$$

$$= |2-2|(6) + |2-3|(12(n + r - 1)) + |3-3|(9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 12n + 12r - 12.$$

$$MHI(CC(n,r)) = \sum_{uv\in E(G)} \left|\left(\frac{1}{2}\right)^{d_u} - \left(\frac{1}{2}\right)^{d_v}\right|$$

$$= \left|\left(\frac{1}{2}\right)^2 - \left(\frac{1}{2}\right)^2\right|(6) + \left|\left(\frac{1}{2}\right)^2 - \left(\frac{1}{2}\right)^3\right|(12(n + r - 1)) + \left|\left(\frac{1}{2}\right)^3 - \left(\frac{1}{2}\right)^3\right|(9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 1.5n + 1.5r - 1.5.$$

$$MMRI(CC(n,r)) = \sum_{uv\in E(G)} \sqrt{\frac{\min(d_u,d_v)}{\max(d_u,d_v)}}$$

$$= \sqrt{\frac{\min(2,2)}{\max(2,2)}}(6) + \sqrt{\frac{\min(2,3)}{\max(2,3)}}(12(n + r - 1)) + \sqrt{\frac{\min(3,3)}{\max(3,3)}}(9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 9n^2 - 9r^2 - 5.202n - 5.202r + 2.202.$$

$$MMRDI(CC(n,r)) = \sum_{uv\in E(G)} \sqrt{\frac{\max(d_u,d_v)}{\min(d_u,d_v)}}$$

$$= \sqrt{\frac{\max(2,2)}{\min(2,2)}}(6) + \sqrt{\frac{\max(2,3)}{\min(2,3)}}(12(n + r - 1)) + \sqrt{\frac{\max(3,3)}{\min(3,3)}}(9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 9n^2 - 9r^2 - 0.3031n - 0.3031r - 2.6969.$$

$$MMDI(CC(n,r)) = \sum_{uv\in E(G)} \frac{\max(d_u,d_v)}{\min(d_u,d_v)}$$

$$= \frac{\max(2,2)}{\min(2,2)}(6) + \frac{\max(2,3)}{\min(2,3)}(12(n + r - 1)) + \frac{\max(3,3)}{\min(3,3)}(9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 9n^2 - 9r^2 + 3n + 3r - 6.$$

$$MMSDI(CC(n,r)) = \sum_{uv\in E(G)} \left(\frac{\max(d_u,d_v)}{\min(d_u,d_v)}\right)^2$$

$$= \left(\frac{\max(2,2)}{\min(2,2)}\right)^2(6) + \left(\frac{\max(2,3)}{\min(2,3)}\right)^2(12(n + r - 1)) + \left(\frac{\max(3,3)}{\min(3,3)}\right)^2(9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 9n^2 - 9r^2 + 12n + 12r - 15.$$

$$SDDI(CC(n,r)) = \sum_{uv\in E(G)} \frac{\min(d_u,d_v)}{\max(d_u,d_v)} + \frac{\max(d_u,d_v)}{\min(d_u,d_v)}$$

$$= \left[\frac{\min(2,2)}{\max(2,2)} + \frac{\max(2,2)}{\min(2,2)}\right](6) + \left[\frac{\min(2,3)}{\max(2,3)} + \frac{\max(2,3)}{\min(2,3)}\right](12(n + r - 1)) + \left[\frac{\min(3,3)}{\max(3,3)} + \frac{\max(3,3)}{\min(3,3)}\right](9n^2 - 9r^2 - 15n - 15r + 6)$$

$$= 18n^2 - 18r^2 - 4n - 4r - 2.$$

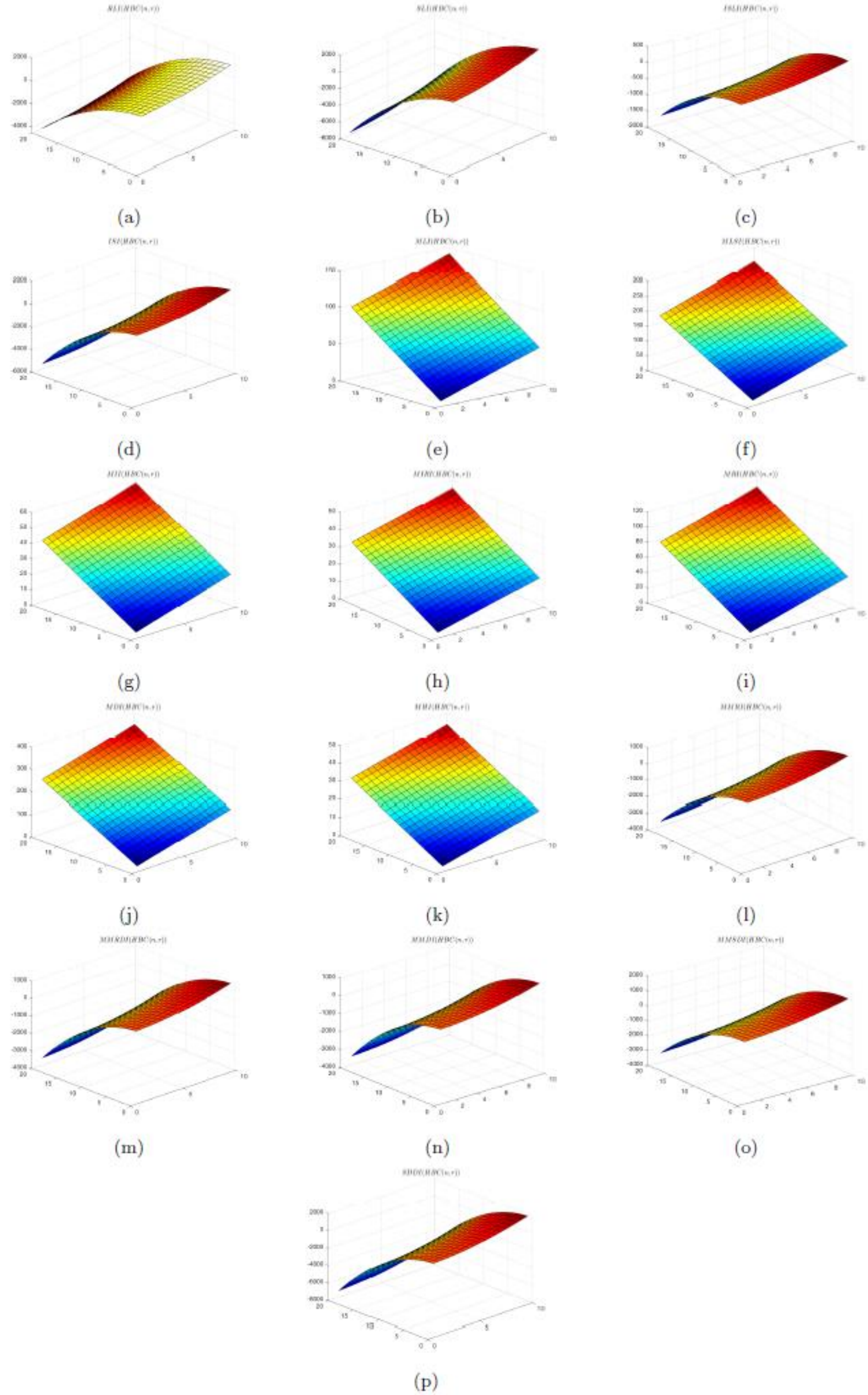

Figure 2: Graphical representation of molecular descriptors of circumcoronene nanostructures with cavity

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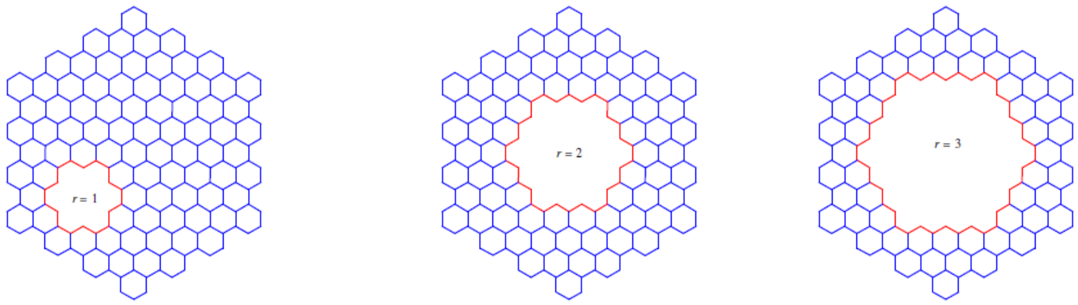
4. Hexa-Peri-Hexabenzocoronene with Cavity $HBC(n,r)$

In this section we find an Adriatic indices of $HBC(n,r)$. There are $27n^2 - 33n - 12r + 18$, vertices and $27n^2 - 9r^2 - 33n - 3r + 12$ edges of $HBC(n)$ respectively see in Figure 3. The edges of $HBC(n,r)$ is classified into three types based on their end vertices degrees as shown in Table 2. The edges of $(2,2)$ has both end vertices of degree 2 and there are $6n$ such edges. Similarly, $(2,3)$ edges has the one end degree 2 and the other end degree 3. This type has $12(n + r - 1)$ edges. If we subtract these two types from the total number of edges, we get the count for $(3,3)$ which is $27n^2 - 9r^2 - 51n - 15r + 24$. Here n denotes the order of HBC and r denotes the size of the cavity.



(a) (b) (c)

Figure 3: (a) $HBC(4)(r = 1)$; (b) $HBC(4)(r = 2)$; (b) $HBC(4)(r = 3)$

Table 2: The edge partition of hexa-peri-hexabenzocoronene with cavity $HBC(n,r)$

(d_u, d_v)	Number of edges in $HBC(n,r)$
(2,2)	$6n$
(2,3)	$12(n + r - 1)$
(3,3)	$27n^2 - 9r^2 - 51n - 15r + 24$

Since this molecular graph has no pendant vertices the edge partition is restricted to only threeclasses. Else, we would have more partition of edges and that will effect in the values of TIs.

Theorem 2. Let G be a $HBC(n,r)$, then

$(i) RLI\big(HBC(n,r)\big) = 32.5876n^2 - 10.8625r^2 - 49.5337n - 8.9662r + 19.8288.$

$(ii) SLI\big(HBC(n,r)\big) = 56.5999n^2 - 18.8666r^2 - 74.3519n - 8.876r + 27.7426.$

$(iii) ISLI\big(HBC(n,r)\big) = 12.8799n^2 - 4.2933r^2 - 14.3446n - 0.7749r + 5.0682.$

$(iv) ISI\big(HBC(n,r)\big) = 40.5n^2 - 13.5r^2 - 56.1n - 8.1r + 21.6.$

$(v)\ MLI(HBC(n,r)) = 4.8656n + 4.8656r - 4.8656.$

$(vi)\ MLSI(HBC(n,r)) = 8.718n + 8.718r - 8.718.$

$(vii)\ MII(HBC(n,r)) = 2n + 2r - 2.$

$(viii)\ MIRI(HBC(n,r)) = 1.5571n + 1.5571r - 1.5571.$

$(ix)\ MRI(HBC(n,r)) = 3.814n + 3.814r - 3.814.$

$(x)\ MDI(HBC(n,r)) = 12n + 12r - 12.$

$(xi)\ MHI(HBC(n,r)) = 1.5n + 1.5r - 1.5.$

$(xii) MMRI\big(HBC(n,r)\big) = 27n^2 - 9r^2 - 35.202n - 5.202r + 14.202.$

$(xiii) MMRDI\big(HBC(n,r)\big) = 27n^2 - 9r^2 - 30.3031n - 0.3031r + 9.3031.$

$(xiv) MMDI\big(HBC(n,r)\big) = 27n^2 - 9r^2 - 27n + 3r + 6.$

$(xv) MMSDI\big(HBC(n,r)\big) = 27n^2 - 9r^2 - 18n + 12r - 3.$

$(xvi) SDDI\big(HBC(n,r)\big) = 54n^2 - 18r^2 - 64n - 4r + 22.$

Proof.

$$RLI(HBC(n,r)) = \sum_{uv\in E(G)} \ln d_G(u) \ln d_G(v)$$

$$= (\ln 2 \times \ln 2)(6n) + (\ln 2 \times \ln 3)(12(n + r - 1)) + (\ln 3 \times \ln 3)(27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 32.5876n^2 - 10.8625r^2 - 49.5337n - 8.9662r + 19.8288.$$

$$SLI(HBC(n,r)) = \sum_{uv\in E(G)} \sqrt{\ln(d_u)} + \sqrt{\ln(d_v)}$$

$$= \left[\sqrt{\ln 2 \times \ln 2}\right](6n) + \left[\sqrt{\ln 2 \times \ln 3}\right](12(n + r - 1)) + \left[\sqrt{\ln 3 \times \ln 3}\right](27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 56.5999n^2 - 18{:}8666r^2 - 74.3519n - 8.876r + 27.7426.$$

$$ISLI(HBC(n,r)) = \sum_{uv\in E(G)} \frac{1}{\sqrt{\ln(d_u)} + \sqrt{\ln(d_v)}}$$

$$= \left[\frac{1}{\sqrt{\ln(2)} + \sqrt{\ln(2)}}\right](6n) + \left[\frac{1}{\sqrt{\ln(2)} + \sqrt{\ln(3)}}\right](12(n + r - 1)) + \left[\frac{1}{\sqrt{\ln(2)} + \sqrt{\ln(3)}}\right](27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 12.8799n^2 - 4.2933r^2 - 14.3446n - 0.7749r + 5.0682.$$

$$ISI(HBC(n,r)) = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u + d_v}$$

$$= \left[\frac{2\times 2}{2+2}\right](6n) + \left[\frac{2\times 3}{2+3}\right](12(n + r - 1)) + \left[\frac{3\times 3}{3+3}\right](27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 40.5n^2 - 13.5r^2 - 56.1n - 8.1r + 21.6.$$

$$MLI(HBC(n,r)) = \sum_{uv\in E(G)} |\ln(d_u) - \ln(d_v)|$$

$$= |\ln(2) - \ln(2)|(6n) + |\ln(2) - \ln(3)|\big(12(n + r - 1)\big) + |\ln(3) - \ln(3)|(27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 4.8656n + 4.8656r - 4.8656.$$

$$MLSI(HBC(n,r)) = \sum_{uv\in E(G)} |\ln^2(d_u) - \ln^2(d_v)|$$

$$= |\ln^2(2) - \ln^2(2)|(6n) + |\ln^2(2) - \ln^2(3)|(12(n + r - 1)) + |\ln^2(3) - \ln^2(3)|(27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 8.718n + 8.718r - 8.718.$$

$$MII(HBC(n,r)) = \sum_{uv\in E(G)} \left|\frac{1}{d_u} - \frac{1}{d_v}\right|$$

$$= \left|\frac{1}{2} - \frac{1}{2}\right|(6n) + \left|\frac{1}{2} - \frac{1}{3}\right|(12(n + r - 1)) + \left|\frac{1}{3} - \frac{1}{3}\right|(27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 2n + 2r - 2.$$

$$MIRI(HBC(n,r)) = \sum_{uv\in E(G)} \left|\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}}\right|$$

$$= \left|\tfrac{1}{\sqrt{2}} - \tfrac{1}{\sqrt{2}}\right|(6n) + \left|\tfrac{1}{\sqrt{2}} - \tfrac{1}{\sqrt{3}}\right|(12(n + r - 1)) + \left|\tfrac{1}{\sqrt{2}} - \tfrac{1}{\sqrt{3}}\right|(27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 1.5571n + 1.5571r - 1.5571.$$

$$MRI(HBC(n,r)) = \sum_{uv\in E(G)} \left|\sqrt{d_u} - \sqrt{d_v}\right|$$

$$= \left|\sqrt{2} - \sqrt{2}\right|(6n) + \left|\sqrt{2} - \sqrt{3}\right|(12(n + r - 1)) + \left|\sqrt{3} - \sqrt{3}\right|(27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 3.814n + 3.814r - 3.814.$$

$$MDI(HBC(n,r)) = \sum_{uv\in E(G)} |d_u - d_v|$$

$$= |2 - 2|(6n) + |2 - 3|(12(n + r - 1)) + |3 - 3|(27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 12n + 12r - 12.$$

$$MHI(HBC(n,r)) = \sum_{uv\in E(G)} \left|\left(\frac{1}{2}\right)^{d_u} - \left(\frac{1}{2}\right)^{d_v}\right|$$

$$= \left|\left(\tfrac{1}{2}\right)^2 - \left(\tfrac{1}{2}\right)^2\right|(6n) + \left|\left(\tfrac{1}{2}\right)^2 - \left(\tfrac{1}{2}\right)^3\right|(12(n + r - 1)) + \left|\left(\tfrac{1}{2}\right)^3 - \left(\tfrac{1}{2}\right)^3\right|(27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 1.5n + 1.5r - 1.5.$$

$$MMRI(HBC(n,r)) = \sum_{uv\in E(G)} \sqrt{\frac{\min(d_u, d_v)}{\max(d_u, d_v)}}$$

$$= \sqrt{\frac{\min(2,2)}{\max(2,2)}}(6n) + \sqrt{\frac{\min(2,3)}{\max(2,3)}}(12(n + r - 1)) + \sqrt{\frac{\min(3,3)}{\max(3,3)}}(27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 27n^2 - 9r^2 - 35.202n - 5.202r + 14.202.$$

$$MMRDI(HBC(n,r)) = \sum_{uv\in E(G)} \sqrt{\frac{\max(d_u, d_v)}{\min(d_u, d_v)}}$$

$$= \sqrt{\frac{\max(2,2)}{\min(2,2)}}(6n) + \sqrt{\frac{\max(2,3)}{\min(2,3)}}(12(n + r - 1)) + \sqrt{\frac{\max(3,3)}{\min(3,3)}}(27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 27n^2 - 9r^2 - 30.3031n - 0.3031r + 9.3031.$$

$$MMDI(HBC(n,r)) = \sum_{uv\in E(G)} \frac{\max(d_u,d_v)}{\min(d_u,d_v)}$$

$$= \frac{\max(2,2)}{\min(2,2)}(6n) + \frac{\max(2,3)}{\min(2,3)}(12(n + r - 1)) + \frac{\max(3,3)}{\min(3,3)}(27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 27n^2 - 9r^2 - 27n + 3r + 6.$$

$$MMSDI(HBC(n,r)) = \sum_{uv\in E(G)} \left(\frac{\max(d_u,d_v)}{\min(d_u,d_v)}\right)^2$$

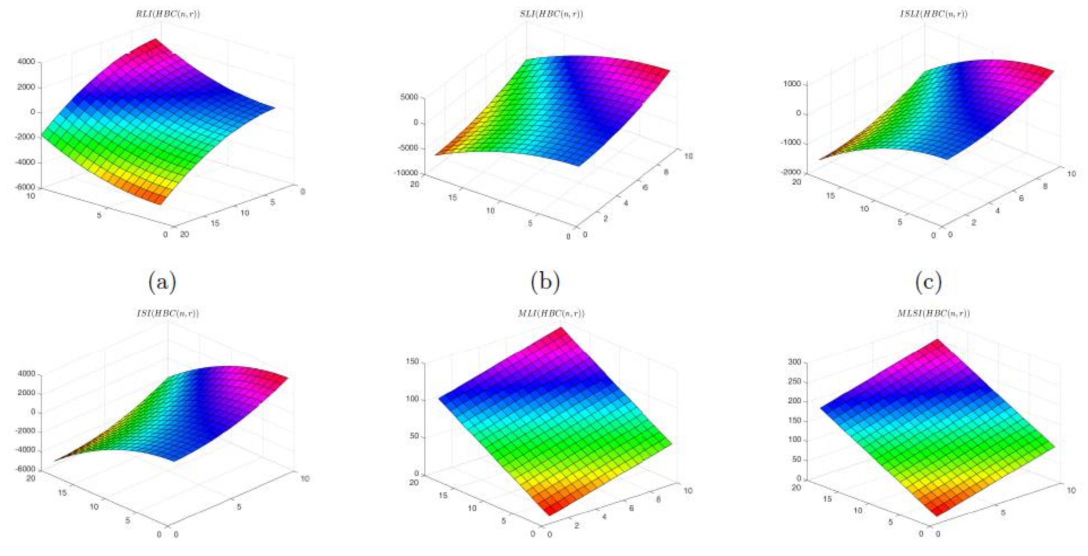
$$= \left(\frac{\max(2,2)}{\min(2,2)}\right)^2(6n) + \left(\frac{\max(2,3)}{\min(2,3)}\right)^2(12(n + r - 1)) + \left(\frac{\max(3,3)}{\min(3,3)}\right)^2(27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 27n^2 - 9r^2 - 18n + 12r - 3.$$

$$SDDI(HBC(n,r)) = \sum_{uv\in E(G)} \frac{\min(d_u,d_v)}{\max(d_u,d_v)} + \frac{\max(d_u,d_v)}{\min(d_u,d_v)}$$

$$= \left[\frac{\min(2,2)}{\max(2,2)} + \frac{\max(2,2)}{\min(2,2)}\right](6n) + \left[\frac{\min(2,3)}{\max(2,3)} + \frac{\max(2,3)}{\min(2,3)}\right](12(n + r - 1)) + \left[\frac{\min(3,3)}{\max(3,3)} + \frac{\max(3,3)}{\min(3,3)}\right](27n^2 - 9r^2 - 51n - 15r + 24)$$

$$= 54n^2 - 18r^2 - 64n - 4r + 22.$$



(a) (b) (c)

(d) (e) (f)

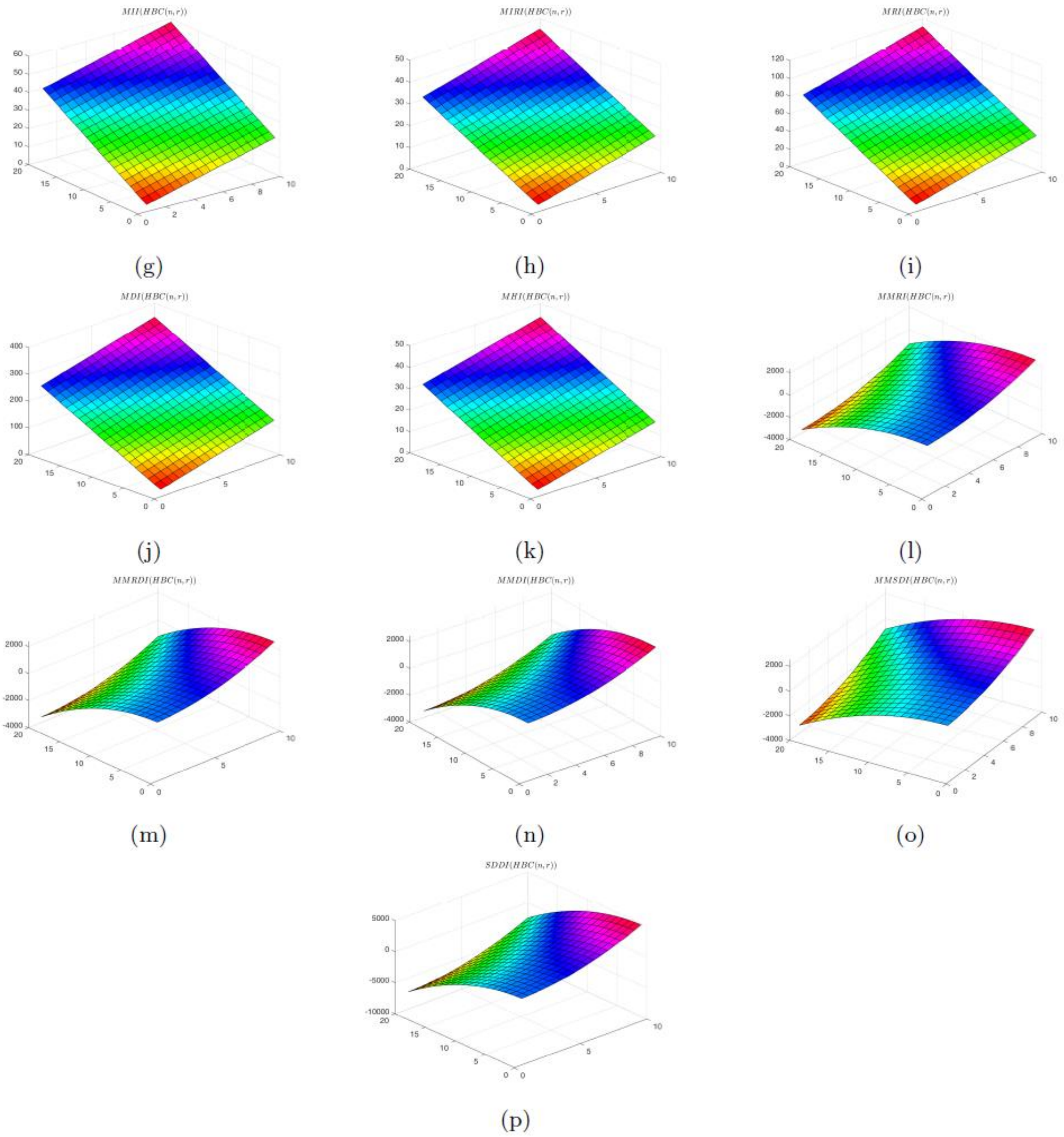


Figure 4: Graphical representation of molecular descriptors of hexa-peri-hexabenzocoronene with cavity

5. Conclusion

This study presents the derivation of precise mathematical formulations for bond additive molecular descriptors pertaining to hexa-peri-hexabenzocoronene with cavity and the circumcoronene series with cavity. A graphical analysis is conducted and presented to illustratethe acquired indices. The use of various methods to compute the several topological indices based on vertex degree offers molecular information. Additionally, this method may be employed for the determination of bond enthalpies, sequential bond energies, and atomizationenergies. It is hypothesised that the topological indices acquired have a significant association with specific physicochemical characteristics, such as the boiling point, as well as structure- property connections. Therefore, our inquiry will contribute to the reduction of laboratory work concerning the aforementioned criteria, as well as aid in preserving the environment through pollution management and the mitigation of air contamination. Furthermore, this study will provide valuable insights into establishing optimal rates for some polycyclic aromatic hydrocarbons (PAHs) that are not artificially produced.

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