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ON VARIOUS DISTANCE-BASED TOPOLOGICAL INDICES OF HEXABENZOCORONENE WITH BITRAPEZIUM STRUCTURE

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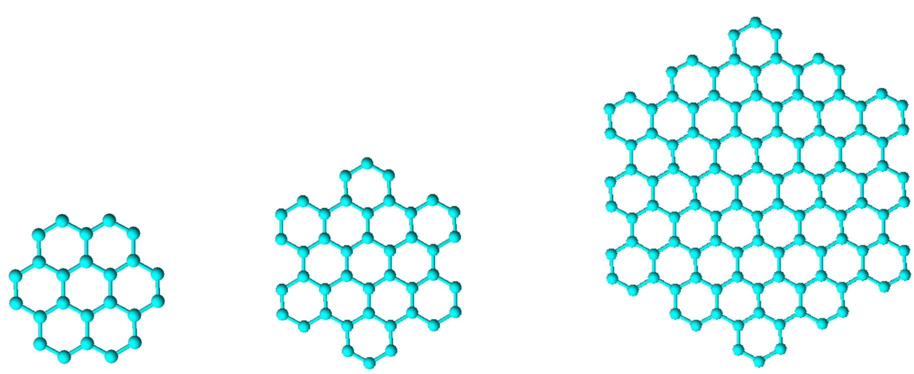
Abstract A molecular descriptor transforms the symbolic depiction of a molecule into a numeric value via a mathematical method, offering a measurable assessment of its chemical properties. Research on these configurations has revealed a strong connection between topological attributes and their physical, chemical, and biological traits. Employing such descriptors enhances our understanding of molecular architectures. In our current research, we employed a theoretical graph-based method to evaluate various distance-related topological descriptors for bitrapezium-shaped hexaperi-hexabenzocoronene with dimensions (p, q, n) where $p < q < n$, when (i) $q - p$ is even and $n - p$ is odd and (ii) $q - p$ is odd and $n - p$ is odd

1 Introduction

Polycyclic aromatic hydrocarbons (PAHs) are a diverse group of organic compounds composed of multiple fused benzene rings[1]. The underlying molecular structures of PAHs significantly influence their chemical behaviours and biological impacts. Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) techniques are computational modelling approaches used to predict the biological activity and physicochemical properties of polycyclic aromatic hydrocarbons (PAHs) based on their molecular structure[2, 3, 4, 5, 6, 7, 8]. Hexa-peri-hexabenzocoronene, commonly referred to as HBC or simply hexabenzocoronene, [9, 10, 11, 12] is a specific kind of polycyclic aromatic hydrocarbon. At its core, there's a central hexagonal ring, reminiscent of benzene, and it's flanked by six other benzene rings, one attached to each side of the central ring, as presented in Figure 1.



(a) (b) (c)

Figure 1: (a) Coronene; (b) Hexa-peri-hexabenzocoronene ($C_{42}H_{18}$) HBC(2); (c) HBC(3).

Topological descriptors, also referred to as molecular descriptors or graph invariants within the realm of molecular modeling, constitute mathematical representations of a molecule's structure derived solely from its topological (graph) arrangement. These indices play a crucial role in theoretically understanding chemical compounds. The Wiener index, first proposed by Harold Wiener in 1947, serves as a fundamental topological descriptor in QSPR and QSAR studies [13]. Defined as the sum of the shortest path lengths between all pairs of vertices in a molecular graph, this index provides a numerical representation of molecular structure, where vertices correspond to atoms and edges represent chemical bonds [14]. Due to its computational simplicity and strong correlation with various molecular properties, the Wiener index has proven particularly useful for predicting the physicochemical and biological characteristics of organic compounds, including polycyclic aromatic hydrocarbons (PAHs).

Expanding on the Wiener index, various distance-based invariants have been introduced for molecular characterization. The Szeged index and its modifications incorporate bond-dependent measures, linking to electrical properties of armchair polyhex carbon nanotubes [15]. The PI index is widely used in QSPR/QSAR studies [16]. These indices play a key role in computational chemistry and molecular modeling.

In this paper, we assess different distance-based topological descriptors for Bitrapezium-shaped HBC of dimensions (p, q, n) with $p \leq q \leq n$, when (i) $q-p$ is even and $n-p$ is odd and (ii) $q-p$ is odd and $n-p$ is odd.

2 Graph-theortical Terminologies

Throughout this paper, our focus is on finite and undirected graphs. Let's consider a molecular graph represented as $G = (V, E)$ with a vertex set $V(G)$ and an edge set $E(G)$. The degree of a vertex $\mu \in V(G)$ is defined as the number of edges incident with it, while the length of the shortest path between vertices μ and ν is denoted as $d_G(\mu, \nu)$. Consequently, the distance between a vertex μ and an edge $f = xy$, denoted by $d_G(\mu, f)$, is given by$min\{d_G(\mu, x), d_G(\mu, y)\}$, and the distance between two edges $e = \mu v$ and $f = xy$, represented as $D_G(e, f)$, is expressed as $min\{d_G(\mu, f), d_G(\nu, f)\}$.

The expressions $N_\mu(e|G)$ and $M_\mu(e|G)$ refer to the set of vertices and edges in graph G that are closer to vertex μ than to vertex ν, with their respective cardinalities denoted as n and m. Similarly, the terms $N_\nu(e|G)$ and $M_\nu(e|G)$ are defined analogously.

The cut technique has proved immensely valuable in handling distance-based graph invariants, establishing them as fundamental concepts in chemical graph theory [17, 18]. This technique involves splitting edges based on the Djoković-Winkler relation Θ, which asserts that for any two edges $e = \mu\nu$ and $f = xy$ in $E(G)$, $d_G(\mu, x) + d_G(\nu, y) \neq d_G(\mu, y) + d_G(\nu, x)$. The notion of the strength-weighted graph was first introduced in [5] and thoroughly explored in subsequent works such as [6, 7, 19, 20, 21, 22, 23, 24, 25] as $G_{sw} = (G, (w_v, s_v), s_e)$ where the vertex-weight capacity and vertex-strength capacity are $w_v : V(G_{sw}) \to \mathbb{R}_0^+$, $s_v : V(G_{sw}) \to \mathbb{R}_0^+$ and the edge-strength capacity $s_e : E(G_{sw}) \to \mathbb{R}_0^+$. Various indices that we studied in this paper are listed below.

(i) **Wiener Type indices:**

$$W(G_{sw}) = \sum_{\{\mu,\nu\} \subseteq V(G_{sw})} w_v(\mu) w_v(\nu) d_{G_{sw}}(\mu, \nu)$$

$$W_e(G_{sw}) = \sum_{\{u,v\} \subseteq V(G_{sw})} s_v(\mu)\, s_v(\nu)\, d_{G_{sw}}(\mu, \nu) + \sum_{\{e,f\} \subseteq E(G_{sw})} s_e(e)\, s_e(f)\, D_{G_{sw}}(e, f)$$
$$+ \sum_{\mu \in V(G_{sw})} \sum_{f \in E(G_{sw})} s_v(\mu)\, s_e(f)\, d_{G_{sw}}(\mu, f)$$

(ii) **Szeged Type Indices:**

$$Sz_v(G_{sw}) = \sum_{e=\mu\nu \in E(G_{sw})} s_e(e) n_\mu(e|G_{sw}) n_\nu(e|G_{sw})$$

$$Sz_e(G_{sw}) = \sum_{e=\mu\nu \in E(G_{sw})} s_e(e) m_\mu(e|G_{sw}) m_\nu(e|G_{sw})$$

(iii) **Degree and Distance-Based Type Index:**

$$S(G_{sw}) = \sum_{\{u,v\} \subseteq V(G_{sw})} \Big[w_v(v)(d_{G_{sw}}(u) + 2s_v(u)) + w_v(u)(d_{G_{sw}}(v) + 2s_v(v)) \Big] d_{G_{sw}}(u,v)$$

$$PI(G_{sw}) = \sum_{e=\mu\nu \in E(G_{sw})} s_e(e) \Big[m_\mu(e|G_{sw}) + m_\nu(e|G_{sw}) \Big]$$

3 Hexabenzocoronene with Bitrapezium structure

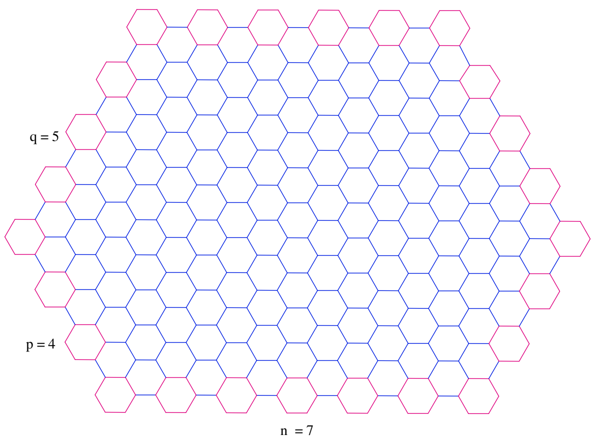


Figure 2: $HBC(4,5,7)$

The investigation into the topological indices of Hexabenzocoronene of dimension n was carried out in [20]. In this section, the precise mathematical formulations for certain notable distance-based topological indices of bitrapezium-shaped hexabenzocoronene with dimensions (p,q,n) a denoted by $HBC(p,q,n)$, are elucidated for two cases, where $p < q < n$. Figure 2 illustrates $HBC(4,5,7)$. The molecular structure of $HBC(p,q,n)$ comprises of $3p^2 - 3q^2 + 6pq - 9p - 3q + 6 + 6n(p+q-1)$ vertices and $(18np - 33p - 11q - 22n + 18nq + 18pq + 9p^2 - 9q^2 + 24)/2$ edges.

Theorem 3.1. *Let G_1 be HBC of dimension p,q,n. Then, the topological descriptors for $p < q < n$,when $q - p$ is even and $n - p$ is odd are,*

(i) $W(G_1) = (-12n^5 + 120n^4q - 30n^4 + 360n^3p^2 + 960n^3pq - 840n^3p - 720n^3q + 480n^3 + 720n^2p^3 + 2880n^2p^2q - 3060n^2p^2 + 720n^2pq^2 - 5040n^2pq + 3780n^2p + 240n^2q^3 - 720n^2q^2 + 2160n^2q - 1410n^2 + 630np^4 + 2760np^3q - 3360np^3 + 540np^2q^2 - 7560np^2q + 6390np^2 - 120npq^3 - 1080npq^2 + 7020npq - 5160np - 270nq^4 + 360nq^3 + 630nq^2 - 2340nq + 1512n + 108p^5 + 720p^4q - 945p^4 + 120p^3q^2 - 2940p^3q + 2790p^3 - 450p^2q^2 + 4410p^2q - 3645p^2 - 300pq^4 + 660pq^3 + 270pq^2 - 3030pq + 2232p + 48q^5 + 165q^4 - 570q^3 + 105q^2 + 792q - 540)/20.$

(ii) $W_e(G_1) = (-324n^5 + 3240n^4q - 990n^4 + 9720n^3p^2 + 25920n^3pq - 27720n^3p - 23760n^3q + 17740n^3 + 19440n^2p^3 + 77760n^2p^2q - 110700n^2p^2 + 19440n^2pq^2 - 185760n^2pq + 169980n^2p + 6480n^2q^3 - 33480n^2q^2 + 114360n^2q - 79740n^2 + 17010np^4 + 74520np^3q - 120600np^3 + 14580np^2q^2 - 278640np^2q + 300060np^2 - 3240npq^3 - 45360npq^2 + 360000npq - 312240np - 7290nq^4 + 21600nq^3 + 18120nq^2 - 152760nq + 115664n + 2916p^5 + 19440p^4q - 33615p^4 + 3240p^3q^2 - 106740p^3q + 125670p^3 - 19710p^2q^2 + 223110p^2q - 215460p^2 - 8100pq^4 +$

$31500pq^3 - 3210pq^2 - 193560pq + 173124p + 1296q^5 + 3015q^4 - 25750q^3 + 17040q^2 + 58144q - 52590)/240$.

(iii) $Sz_v(G_1) = (336n^5 - 240n^4p - 2880n^4q + 1260n^4 + 8640n^3p^3 + 25920n^3p^2q - 29760n^3p^2 + 25920n^3pq^2 - 57600n^3pq + 34560n^3p + 8640n^3q^3 - 18720n^3q^2 + 24480n^3q - 12600n^3 + 12960n^2p^4 + 51840n^2p^3q - 68640n^2p^3 + 51840n^2p^2q^2 - 168480n^2p^2q + 129240n^2p^2 - 77760n^2pq^2 + 168480n^2pq - 101400n^2p - 12960n^2q^4 + 3360n^2q^3 + 40320n^2q^2 - 56640n^2q + 28080n^2 + 6480np^5 + 32400np^4q - 49440np^4 + 38880np^3q^2 - 153600np^3q + 133800np^3 - 12960np^2q^3 - 83520np^2q^2 + 245880np^2q - 168480np^2 - 19440npq^4 + 34560npq^3 + 71640npq^2 - 174000npq + 102720np + 6480nq^5 + 11760nq^4 - 27960nq^3 - 19320nq^2 + 49200nq - 25176n + 1080p^6 + 6480p^5q - 11088p^5 + 9720p^4q^2 - 43440p^4q + 42570p^4 - 4320p^3q^3 - 28320p^3q^2 + 97320p^3q - 76500p^3 - 9720p^2q^4 + 22560p^2q^3 + 34740p^2q^2 - 107460p^2q + 72000p^2 + 6480pq^5 + 9600pq^4 - 35640pq^3 - 13860pq^2 + 61440pq - 36072p - 1080q^6 - 4080q^5 + 510q^4 + 14580q^3 - 1680q^2 - 13920q + 8100)/160$.

(iv) $Sz_e(G_1) = (648n^5 + 2700n^4p - 2160n^4q - 2850n^4 + 29160n^3p^3 + 87480n^3p^2q - 110700n^3p^2 + 87480n^3pq^2 - 234360n^3pq + 141960n^3p + 29160n^3q^3 - 111780n^3q^2 + 159480n^3q - 64280n^3 + 43740n^2p^4 + 174960n^2p^3q - 284040n^2p^3 + 174960n^2p^2q^2 - 741960n^2p^2q + 638190n^2p^2 - 392040n^2pq^2 + 1005660n^2pq - 616170n^2p - 43740n^2q^4 + 58320n^2q^3 + 180990n^2q^2 - 425370n^2q + 217320n^2 + 21870np^5 + 109350np^4q - 197910np^4 + 131220np^3q^2 - 680400np^3q + 676590np^3 - 43740np^2q^3 - 396900np^2q^2 + 1453770np^2q - 1085400np^2 - 65610npq^4 + 228960npq^3 + 288810npq^2 - 1263420npq + 822060np + 21870nq^5 + 25650nq^4 - 151050nq^3 - 40740nq^2 + 385380nq - 237928n + 3645p^6 + 21870p^5q - 42201p^5 + 32805p^4q^2 - 184815p^4q + 195165p^4 - 14580p^3q^3 - 142830p^3q^2 + 572520p^3q - 460680p^3 - 32805p^2q^4 + 143910p^2q^3 + 129600p^2q^2 - 788220p^2q + 573570p^2 + 21870pq^5 + 12015pq^4 - 191460pq^3 + 10650pq^2 + 495000pq - 356694p - 3645q^6 - 13203q^5 + 10665q^4 + 69230q^3 - 33270q^2 - 115682q + 87330)/240$.

(v) $S(G_1) = (-18n^5 + 180n^4q - 50n^4 + 540n^3p^2 + 1440n^3pq - 1400n^3p - 1200n^3q + 840n^3 + 1080n^2p^3 + 4320n^2p^2q - 5100n^2p^2 + 1080n^2pq^2 - 8400n^2pq + 6810n^2p + 360n^2q^3 - 1200n^2q^2 + 4080n^2q - 2770n^2 + 945np^4 + 4140np^3q - 5600np^3 + 810np^2q^2 - 12600np^2q + 11655np^2 - 180npq^3 - 1800npq^2 + 13110npq - 10250np - 405nq^4 + 600nq^3 + 975nq^2 - 4710nq + 3258n + 162p^5 + 1080p^4q - 1575p^4 + 180p^3q^2 - 4900p^3q + 5025p^3 - 750p^2q^2 + 8235p^2q - 7200p^2 - 450pq^4 + 1100pq^3 + 285pq^2 - 6100pq + 4848p + 72q^5 + 275q^4 - 975q^3 + 280q^2 + 1668q - 1260)/5$.

(vi) $PI(G_1) = (12n^3 + 324n^2p^2 + 648n^2pq - 792n^2p + 324n^2q^2 - 864n^2q + 514n^2 + 324np^3 + 972np^2q - 1638np^2 + 324npq^2 - 2556npq + 2484np - 324nq^3 + 54nq^2 + 1456nq - 1168n + 81p^4 + 324p^3q - 594p^3 + 162p^2q^2 - 1494p^2q + 1620p^2 - 324pq^3 + 270pq^2 + 1728pq - 1760p + 81q^4 + 186q^3 - 350q^2 - 572q + 650)/4$.

Proof. Let $\{V_{1i} : 1 \le i \le p\}$, $\{V_{2i} : 1 \le i \le (q-p)/2\}$, $\{V_{3i} : 1 \le i \le (q-p)/2\}$, $\{V_{4i} : 1 \le i \le n-q+p-1\}$, $\{V_{5i} : 1 \le i \le n-q+p-2\}$, $\{V'_{1i} : 1 \le i \le p\}$, $\{V'_{2i} : 1 \le i \le (q-p)/2\}$ and $\{V'_{3i} : 1 \le i \le (q-p)/2\}$ be the vertical cuts. Also, let $\{A_{1i} : 1 \le i \le n-q+p\}$, $\{A_{2i} : 1 \le i \le (2q-n-p+1)/2\}$, $\{A_{3i} : 1 \le i \le (2q-n-p-1)/2\}$, $\{A_{4i} : 1 \le i \le 2p-3\}$, $\{A_{5i} : 1 \le i \le (n-p+1)/2\}$, $\{A_{6i} : 1 \le i \le (n-p-1)/2\}$ and $\{A_{7i} : 1 \le i \le p\}$ be the various acute cuts of the $HBC(p,q,n)$ as shown in Figure 3 and Figure 5. The quotient graphs G_1/V_{1i}, G_1/V_{2i}, G_1/V_{3i}, G_1/V_{4i}, G_1/V_{5i}, G_1/A_{1i}, G_1/A_{2i}, G_1/A_{3i}, G_1/A_{4i}, G_1/A_{5i}, G_1/A_{6i} and G_1/A_{7i} are K_2 graph as sketched in Figure 4 and 6 along with their edge strengths and corresponding vertex strength weighted values are given in Table 1. We proceed to compute the different topological indices as follows, using the same principles as for obtuse cuts:

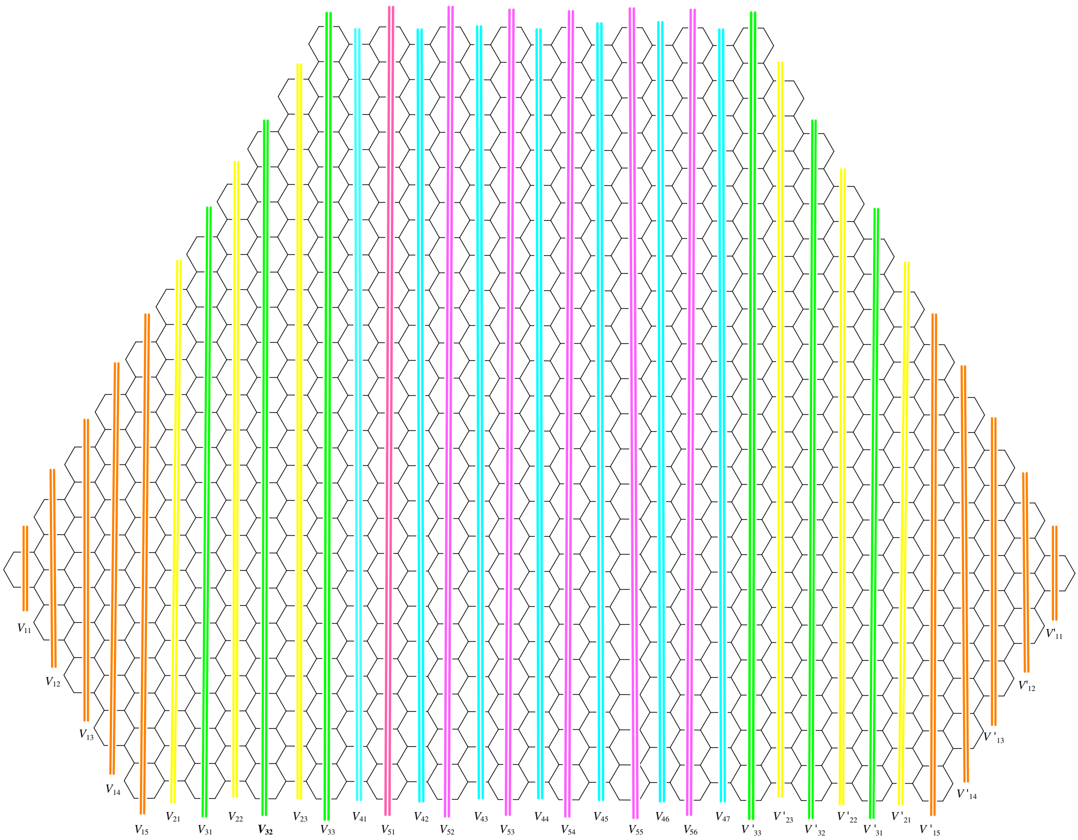


Figure 3: Vertical cuts

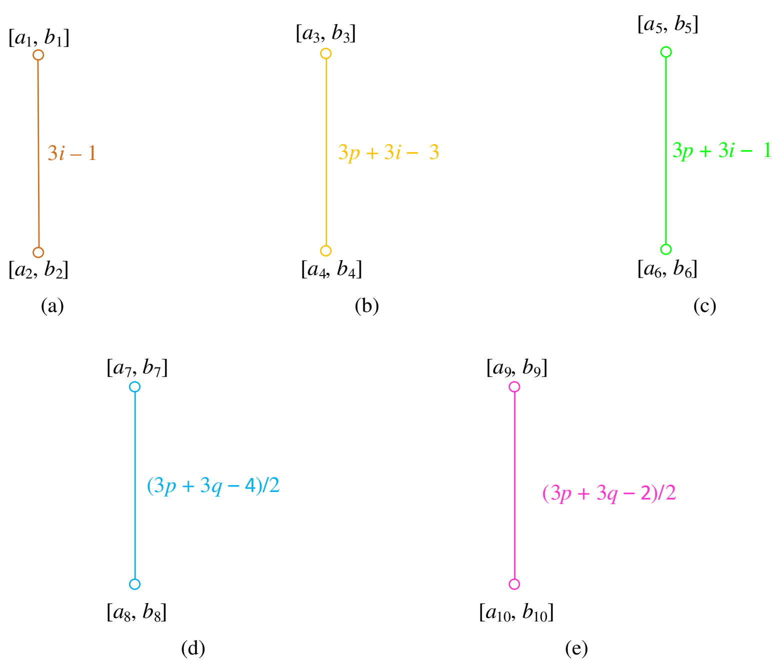


Figure 4: (a) $\{G_1/V_{1i} : 1 \leq i \leq p\}$; (b) $\{G_1/V_{2i} : 1 \leq i \leq (q-p)/2\}$; (c) $\{G_1/V_{3i} : 1 \leq i \leq (q-p)/2\}$; (d) $\{G_1/V_{4i} : 1 \leq i \leq n-q+p-1\}$; (e) $\{G_1/V_{5i} : 1 \leq i \leq n-q+p-2\}$

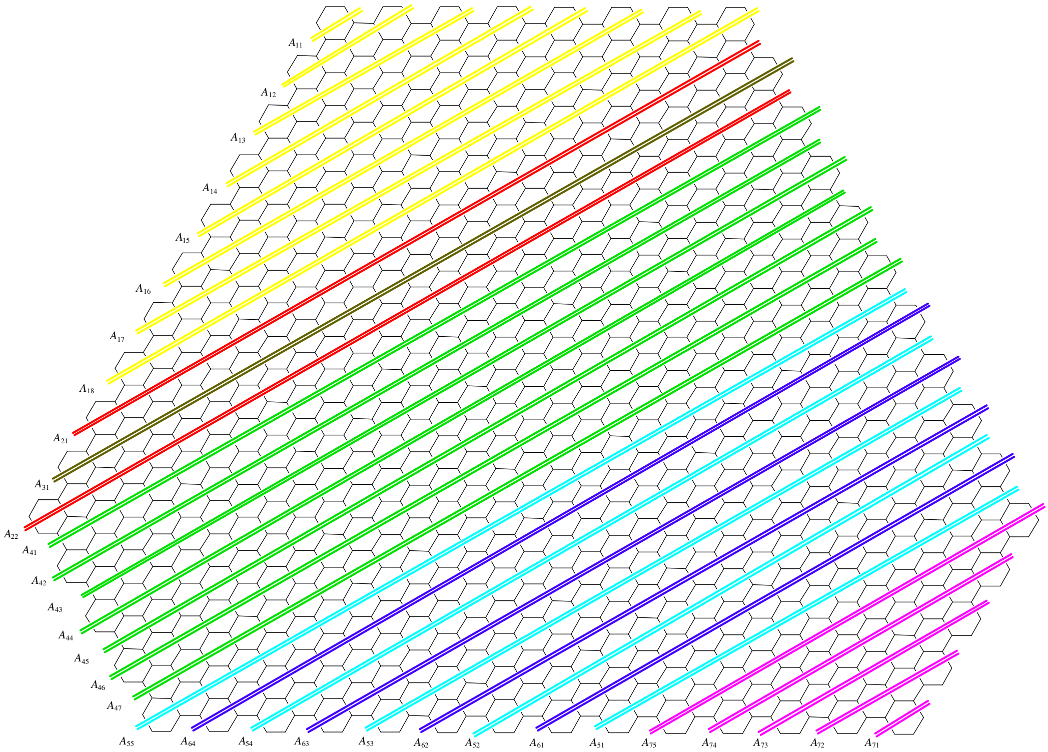


Figure 5: Acute cuts

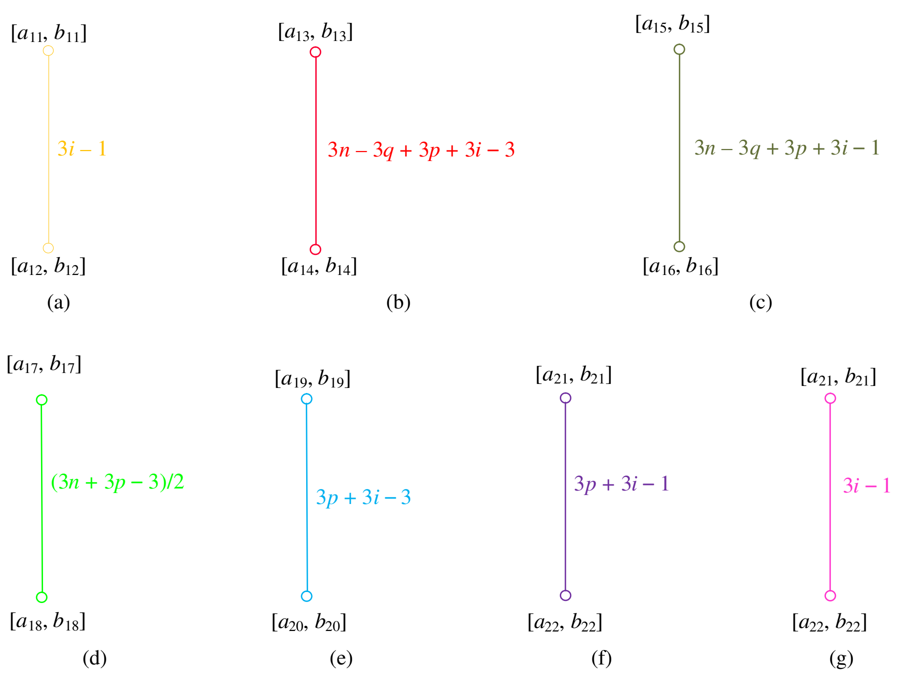


Figure 6: (a) $\{G_1/A_{1i} : 1 \leq i \leq n - q + p\}$; (b) $\{G_1/A_{2i} : 1 \leq i \leq (2q - n - p + 1)/2\}$; (c) $\{G_1/A_{3i} : 1 \leq i \leq (2q - n - p - 1)/2\}$; (d) $\{G_1/A_{4i} : 1 \leq i \leq 2p - 3\}$; (e) $\{G_1/A_{5i} : 1 \leq i \leq (n - p + 1)/2\}$; (f) $\{G_1/A_{6i} : 1 \leq i \leq (n - p - 1)/2\}$; (g) $\{G_1/A_{7i} : 1 \leq i \leq p\}$

Table 1: Vertex strength weighted values for $p < q < n,\ q-p$ is even and $n-p$ is odd

Quotient Graph Component Values
G_1/V_{1i}: $1 \leq i \leq p$; $ev_{1i} = 3i - 1$
$a_1 = 3i^2$; $a_2 = N - a_1$ $b_1 = (9i^2 - 7i + 2)/2$; $b_2 = M - b_1 - ev_{1i}$
G_1/V_{2i}: $1 \leq i \leq (q-p)/2$; $ev_{2i} = 3p + 3i - 3$
$a_3 = 3p^2 + (2i-1)(6p + 3i - 3)$; $a_4 = N - a_3$ $b_3 = (18i^2 + 36ip - 36i + 9p^2 - 25p + 16)/2$; $b_4 = M - b_3 - ev_{2i}$
G_1/V_{3i}: $1 \leq i \leq (q-p)/2$; $ev_{3i} = 3p + 3i - 1$
$a_5 = 3p^2 + 12pi + 3i(2i-1)$; $a_6 = N - a_5$ $b_5 = (18i^2 + 36ip - 18i + 9p^2 - 7p + 2)/2$; $b_6 = M - b_5 - ev_{3i}$
G_1/V_{4i}: $1 \leq i \leq (n - q + p - 1)$; $ev_{4i} = (3p + 3q - 4)/2$
$a_7 = (12ip - 3p - 9q - 12i + 12iq + 6pq - 3p^2 + 3q^2 + 6)/2$; $a_8 = N - a_7$ $b_7 = (4p - 18q + 18pq + 2i(9p + 9q - 11) - 9p^2 + 9q^2 + 5)/4$; $b_8 = M - b_7 - ev_{4i}$
G_1/V_{5i}: $1 \leq i \leq (n - q + p - 2)$; $ev_{5i} = (3p + 3q - 2)/2$
$a_9 = (3p - 12i - 3q + 12ip + 12iq + 6pq - 3p^2 + 3q^2)/2$; $a_{10} = N - a_9$ $b_9 = (4p - 44i - 18q + 36ip + 36iq + 36pq - 18p^2 + 9(p-q)^2 + 4)/4$; $b_{10} = M - b_9 - ev_{5i}$
G_1/A_{1i}: $1 \leq i \leq n - q + p$; $ea_{1i} = 3i - 1$
$a_{11} = 3i^2$; $a_{12} = N - a_{11}$ $b_{11} = (9i^2 - 7i + 2)/2$; $b_{12} = M - b_{11} - ea_{1i}$
G_1/A_{2i}: $1 \leq i \leq (2q - n - p + 1)/2$; $ea_{2i} = 3(n - q + p + i - 1)$
$a_{13} = 3(n - q + p)^2 + (2i-1)(6n - 6q + 6p + 3i - 3)$; $a_{14} = N - a_{13}$ $b_{13} = (25q - 25n - 25p - 36i + 9(n + p - q)^2 + 2i(18n + 18p - 18q) + 18i^2 + 16)/2$; $b_{14} = M - b_{13} - ea_{2i}$
G_1/A_{3i}: $1 \leq i \leq (2q - n - p - 1)/2$; $ea_{3i} = 3(n - q + p + i) + 1$
$a_{15} = 3(n - q + p)^2 + 12(n - q + p)i + 3i(2i - 1)$; $a_{16} = N - a_{15}$ $b_{15} = (7q - 7n - 7p - 18i + 9(n + p - q)^2 + 2i(18n + 18p - 18q) + 18i^2 + 2)/2$; $b_{16} = M - b_{15} - ea_{3i}$
G_1/A_{4i}: $1 \leq i \leq 2p - 3$; $ea_{4i} = (3n + 3p - 3)/2$
$a_{17} = (3p - 3n - 6i + 6in + 6ip + 6np + 3n^2 - 3p^2)/2$; $a_{18} = N - a_{17}$ $b_{17} = (4p - 18n - 22i + 18in + 18ip + 18np + 9n^2 - 9p^2 + 5)/4$; $b_{18} = M - b_{17} - ea_{4i}$
G_1/A_{5i}:$1 \leq i \leq (n - p + 1)/2$; $ea_{5i} = (3p + 3i - 3)$
$a_{19} = 3p^2 + (2i-1)(6p + 3i - 3)$; $a_{20} = N - a_{19}$ $b_{19} = (18i^2 + 36ip - 36i + 9p^2 - 25p + 16)/2$; $b_{20} = M - b_{19} - ea_{5i}$
G_1/A_{6i}: $1 \leq i \leq (n - p - 1)/2$; $ea_{6i} = 3p + 3i - 1$
$a_{21} = 3p^2 + 12pi + 3i(2i-1)$; $a_{22} = N - a_{21}$ $b_{21} = (18i^2 + 36ip - 18i + 9p^2 - 7p + 2)/2$; $b_{22} = M - b_{21} - ea_{6i}$
G_1/A_{7i}: $1 \leq i \leq p$; $ea_{7i} = 3i - 1$
$a_{23} = 3i^2$; $a_{24} = N - a_{23}$ $b_{23} = (9i^2 - 7i + 2)/2$; $b_{24} = M - b_{23} - ea_{7i}$

Following the computational procedure adopted in [5, 26], we present the values of various distance-based topological indices of $HBC(p, q, n)$, for the case $p < q < n$, $q - p$ even and $n - p$ odd.

□

Theorem 3.2. *Let G_2 be HBC of dimension p, q, n. Then, the topological descriptors for $p < q < n$, when $q - p$ is odd and $n - p$ is odd are,*

(i) $W(G_2) = (-12n^5 + 120n^4q - 30n^4 + 360n^3p^2 + 960n^3pq - 840n^3p - 720n^3q + 480n^3 + 720n^2p^3 + 2880n^2p^2q - 3060n^2p^2 + 720n^2pq^2 - 5040n^2pq + 3780n^2p + 240n^2q^3 - 720n^2q^2 + 2160n^2q - 1410n^2 + 630np^4 + 2760np^3q - 3360np^3 + 540np^2q^2 - 7560np^2q + 6390np^2 - 120npq^3 - 1080npq^2 + 7020npq - 5160np - 270nq^4 + 360nq^3 + 630nq^2 - 2340nq + 1512n + 108p^5 + 720p^4q - 945p^4 + 120p^3q^2 - 2940p^3q + 2790p^3 - 450p^2q^2 + 4410p^2q - 3645p^2 - 300pq^4 + 660pq^3 + 270pq^2 - 3030pq + 2232p + 48q^5 + 165q^4 - 570q^3 + 105q^2 + 792q - 540)/20.$

(ii) $W_e(G_2) = (-324n^5 + 3240n^4q - 990n^4 + 9720n^3p^2 + 25920n^3pq - 27720n^3p - 23760n^3q + 17740n^3 + 32400n^2p^3 + 77760n^2p^2q - 194940n^2p^2 + 19440n^2pq^2 - 185760n^2pq + 319020n^2p + 6480n^2q^3 - 33480n^2q^2 + 114360n^2q - 157500n^2 + 51570np^4 + 48600np^3q - 378360np^3 + 14580np^2q^2 - 110160np^2q + 912780np^2 - 3240npq^3 - 45360npq^2 + 61920npq - 900480np - 7290nq^4 + 21600nq^3 + 18120nq^2 + 2760nq + 314354n + 36p^5 - 6480p^4q + 17745p^4 + 16200p^3q^2 + 77580p^3q - 156090p^3 - 103950p^2q^2 - 177930p^2q + 414300p^2 - 8100pq^4 + 31500pq^3 + 145830pq^2 + 144120pq - 442266p + 1296q^5 + 3015q^4 - 25750q^3 - 60720q^2 - 36866q + 166275)/240.$

(iii) $Sz_v(G_2) = (336n^5 - 240n^4p - 2880n^4q + 1260n^4 + 8640n^3p^3 + 25920n^3p^2q - 29760n^3p^2 + 25920n^3pq^2 - 57600n^3pq + 34560n^3p + 8640n^3q^3 - 18720n^3q^2 + 24480n^3q - 12600n^3 + 12960n^2p^4 + 51840n^2p^3q - 68640n^2p^3 + 51840n^2p^2q^2 - 168480n^2p^2q + 129240n^2p^2 - 77760n^2pq^2 + 168480n^2pq - 101400n^2p - 12960n^2q^4 + 3360n^2q^3 + 40320n^2q^2 - 56640n^2q + 28080n^2 + 6480np^5 + 32400np^4q - 49440np^4 + 38880np^3q^2 - 153600np^3q + 133800np^3 - 12960np^2q^3 - 83520np^2q^2 + 245880np^2q - 168480np^2 - 19440npq^4 + 34560npq^3 + 71640npq^2 - 174000npq + 102360np + 6480nq^5 + 11760nq^4 - 27960nq^3 - 19320nq^2 + 48840nq - 24816n + 1080p^6 + 6480p^5q - 11088p^5 + 9720p^4q^2 - 43440p^4q + 42570p^4 - 4320p^3q^3 - 28320p^3q^2 + 97320p^3q - 76500p^3 - 9720p^2q^4 + 22560p^2q^3 + 34740p^2q^2 - 107460p^2q + 71640p^2 + 6480pq^5 + 9600pq^4 - 35640pq^3 - 13860pq^2 + 61440pq - 35532p - 1080q^6 - 4080q^5 + 510q^4 + 14580q^3 - 1320q^2 - 14100q + 7830)/160.$

(iv) $Sz_e(G_2) = (648n^5 + 2700n^4p - 2160n^4q - 2850n^4 + 48600n^3p^3 + 87480n^3p^2q - 237060n^3p^2 + 87480n^3pq^2 - 234360n^3pq + 365520n^3p + 29160n^3q^3 - 111780n^3q^2 + 159480n^3q - 180920n^3 + 115020n^2p^4 + 136080n^2p^3q - 816480n^2p^3 + 174960n^2p^2q^2 - 489240n^2p^2q + 1907190n^2p^2 - 392040n^2pq^2 + 558540n^2pq - 1838190n^2p - 43740n^2q^4 + 58320n^2q^3 + 180990n^2q^2 - 191550n^2q + 631380n^2 + 69390np^5 + 31590np^4q - 559350np^4 + 150660np^3q^2 - 112320np^3q + 1559670np^3 - 43740np^2q^3 - 523260np^2q^2 + 152370np^2q - 1941390np^2 - 65610npq^4 + 228960npq^3 + 512370npq^2 - 75960npq + 1077000np + 21870nq^5 + 25650nq^4 - 151050nq^3 - 158190nq^2 + 9060nq - 206008n - 675p^6 - 17010p^5q + 39159p^5 + 52245p^4q^2 + 130545p^4q - 304515p^4 - 14580p^3q^3 - 288630p^3q^2 - 305520p^3q + 906870p^3 - 32805p^2q^4 + 143910p^2q^3 + 479520p^2q^2 + 320130p^2q - 1296045p^2 + 21870pq^5 + 12015pq^4 - 191460pq^3 - 330360pq^2 - 153150pq + 896451p - 3645q^6 - 13203q^5 + 10665q^4 + 69500q^3 + 84645q^2 + 24973q - 241245)/240.$

(v) $S(G_2) = (-18n^5 + 180n^4q - 50n^4 + 540n^3p^2 + 1440n^3pq - 1400n^3p - 1200n^3q + 840n^3 + 1440n^2p^3 + 4320n^2p^2q - 7440n^2p^2 + 1080n^2pq^2 - 8400n^2pq + 10950n^2p + 360n^2q^3 - 1200n^2q^2 + 4080n^2q - 4930n^2 + 1905np^4 + 3420np^3q - 12680np^3 + 810np^2q^2 - 7920np^2q + 28155np^2 - 180npq^3 - 1800npq^2 + 4830npq - 25670np - 405nq^4 + 600nq^3 + 975nq^2 - 390nq + 8298n + 402p^5 + 360p^4q - 3855p^4 + 540p^3q^2 + 140p^3q + 12945p^3 - 3090p^2q^2 - 2385p^2q - 20040p^2 - 450pq^4 + 1100pq^3 + 4425pq^2 + 2360pq + 14688p + 72q^5 + 275q^4 - 975q^3 - 1880q^2 - 492q - 4140)/5.$

(vi) $PI(G_2) = (12n^3 + 324n^2p^2 + 648n^2pq - 792n^2p + 324n^2q^2 - 864n^2q + 514n^2 + 324np^3 + 972np^2q - 1638np^2 + 324npq^2 - 2556npq + 2484np - 324nq^3 + 54nq^2 + 1456nq - 1166n + 81p^4 + 324p^3q - 594p^3 + 162p^2q^2 - 1494p^2q + 1620p^2 - 324pq^3 + 270pq^2 + 1728pq - 1758p + 81q^4 + 186q^3 - 350q^2 - 574q + 651)/4.$

Proof. Let $\{V_{1i} : 1 \le i \le p\}$, $\{V_{2i} : 1 \le i \le (q-p+1)/2\}$, $\{V_{3i} : 1 \le i \le (q-p-1)/2\}$, $\{V_{4i} : 1 \le i \le 2n-2q+2p-3\}$, $\{V'_{1i} : 1 \le i \le p\}$, $\{V'_{2i} : 1 \le i \le (q-p+1)/2\}$ and $\{V'_{3i} : 1 \le i \le (q-p-1)/2\}$ be the vertical cuts. Also, let $\{A_{1i} : 1 \le i \le n-q+p\}$,

$\{A_{2i} : 1 \leq i \leq (2q-n-p+1)/2\}$, $\{A_{3i} : 1 \leq i \leq (2q-n-p-1)/2\}$, $\{A_{4i} : 1 \leq i \leq 2p-3\}$, $\{A_{5i} : 1 \leq i \leq (n-p+1)/2\}$, $\{A_{6i} : 1 \leq i \leq (n-p-1)/2\}$ and $\{A_{7i} : 1 \leq i \leq p\}$ be the various acute cuts of the $HBC(p,q,n)$ as shown in Figure 7 and 9. The quotient graphs G_2/V_{1i}, G_2/V_{2i}, G_2/V_{3i}, G_2/V_{4i}, G_2/V_{5i}, G_2/A_{1i}, G_2/A_{2i}, G_2/A_{3i}, G_2/A_{4i}, G_2/A_{5i}, G_2/A_{6i} and G_2/A_{7i} are K_2 graph as sketched in Figure 8 and 10 along with their edge strengths and corresponding vertex strength weighted values are given in Table 2. We proceed to compute the different topological indices as follows, using the same principles as for obtuse cuts:

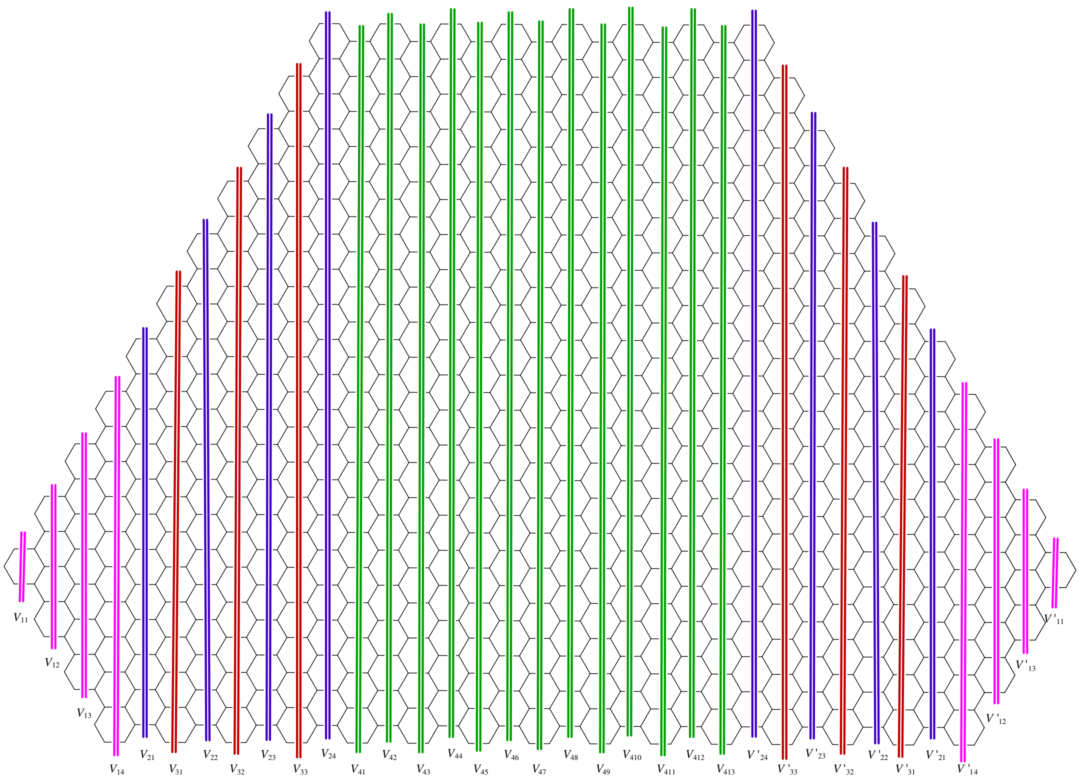


Figure 7: Vertical cuts

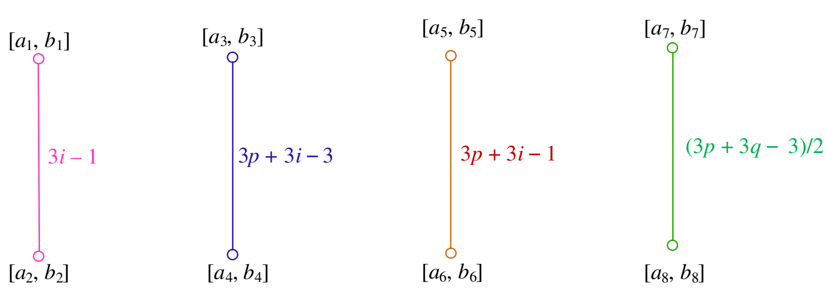


Figure 8: (a) $\{G_2/V_{1i} : 1 \leq i \leq p\}$; (b) $\{G_2/V_{2i} : 1 \leq i \leq (q-p+1)/2\}$; (c) $\{G_2/V_{3i} : 1 \leq i \leq (q-p-1)/2\}$; (d) $\{G_2/V_{4i} : 1 \leq i \leq 2n-2q+2p-3\}$

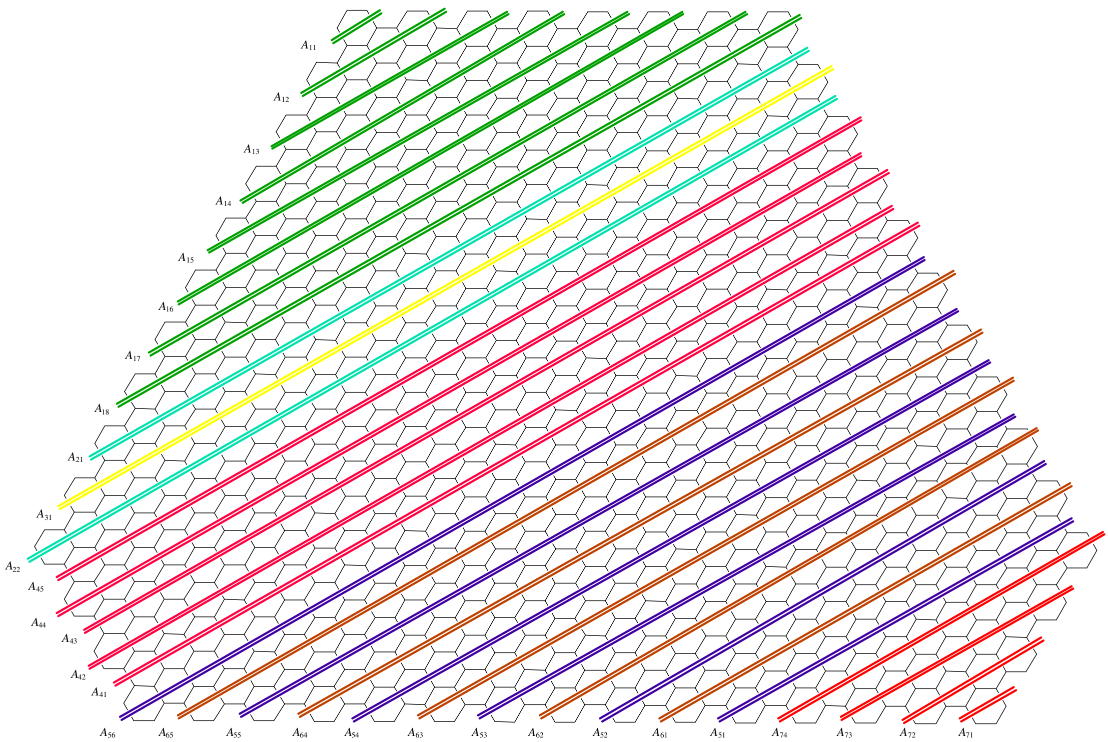


Figure 9: Acute cuts

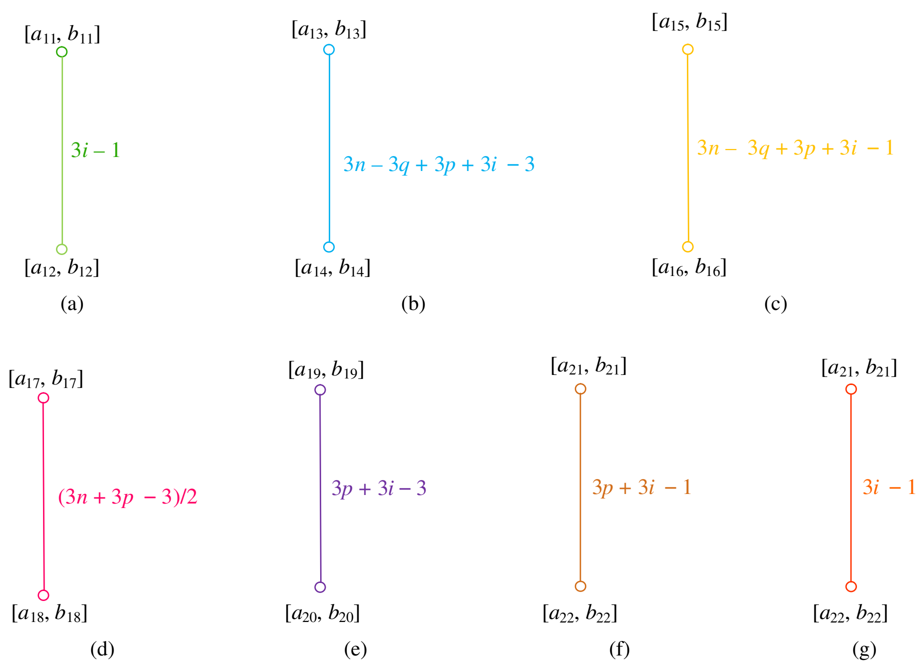


Figure 10: (a) $\{G_2/A_{1i} : 1 \leq i \leq n-q+p\}$; (b) $\{G_2/A_{2i} : 1 \leq i \leq (2q-n-p+1)/2\}$; (c) $\{G_2/A_{3i} : 1 \leq i \leq (2q-n-p-1)/2\}$; (d) $\{G_2/A_{4i} : 1 \leq i \leq 2p-3\}$; (e) $\{G_2/A_{5i} : 1 \leq i \leq (n-p+1)/2\}$; (f) $\{G_2/A_{6i} : 1 \leq i \leq (n-p-1)/2\}$; (g) $\{G_2/A_{7i} : 1 \leq i \leq p\}$

Table 2: Vertex strength weighted values for $p < q < n,\ q - p$ is odd and $n - p$ is odd

Quotient Graph Component Values
G_2/V_{1i}: $1 \leq i \leq p$; $ev_{1i} = 3i - 1$
$a_1 = 3i^2$; $a_2 = N - a_1$ $b_1 = (9i^2 - 7i + 2)/2$; $b_2 = M - b_1 - ev_{1i}$
G_2/V_{2i}:$1 \leq i \leq (q - p + 1)/2$; $ev_{2i} = 3p + 3i - 3$
$a_3 = 3p^2 + (2i - 1)(6p + 3i - 3)$; $a_4 = N - a_3$ $b_3 = (18i^2 + 36ip - 36i + 9p^2 - 25p + 16)/2$; $b_4 = M - b_3 - ev_{2i}$
G_2/V_{3i}:$1 \leq i \leq (q - p - 1)/2$; $ev_{3i} = 3p + 3i - 1$
$a_5 = 3p^2 + 12pi + 3i(2i - 1)$; $a_6 = N - a_5$ $b_5 = (18i^2 + 36ip - 18i + 9p^2 - 7p + 2)/2$; $b_6 = M - b_5 - ev_{3i}$
G_2/V_{4i}: $1 \leq i \leq 2n - 2q + 2p - 3$; $ev_{4i} = (3p + 3q - 3)/2$
$a_7 = 3p^2 + 6p(q - p) + 3(q - p)(q - p - 1)/2 + 3i(p + q - 1)$; $a_8 = N - a_7$ $b_7 = (4p - 18q + 18pq + 2i(9p + 9q - 11) - 9p^2 + 9q^2 + 5)/4$; $b_8 = M - b_7 - ev_{4i}$
G_2/A_{1i}: $1 \leq i \leq n - q + p$; $ea_{1i} = 3i - 1$
$a_9 = 3i^2$; $a_{10} = N - a_9$ $b_9 = (9i^2 - 7i + 2)/2$; $b_{10} = M - b_9 - ea_{1i}$
G_2/A_{2i}: $1 \leq i \leq (2q - n - p + 1)/2$; $ea_{2i} = 3n - 3q + 3p + 3i - 3$
$a_{11} = 3(n - q + p)^2 + (2i - 1)(6n - 6q + 6p + 3i - 3)$; $a_{12} = N - a_{11}$ $b_{11} = (25q - 25n - 25p - 36i + 9(n + p - q)^2 + 2i(18n + 18p - 18q) + 18i^2 + 16)/2$; $b_{12} = M - b_{11} - ea_{2i}$
G_2/A_{3i}: $1 \leq i \leq (2q - n - p - 1)/2$; $ea_{3i} = 3n - 3q + 3p + 3i - 1$
$a_{13} = 3(n - q + p)^2 + 12(n - q + p)i + 3i(2i - 1)$; $a_{14} = N - a_{13}$ $b_{13} = (7q - 7n - 7p - 18i + 9(n + p - q)^2 + 2i(18n + 18p - 18q) + 18i^2 + 2)/2$; $b_{14} = M - b_{13} - ea_{3i}$
G_2/A_{4i}: $1 \leq i \leq 2p - 3$; $ea_{4i} = (3n + 3p - 2)/2$
$a_{15} = (3p - 3n - 6i + 6in + 6ip + 6np + 3n^2 - 3p^2)/2$; $a_{16} = N - a_{15}$ $b_{15} = (26i - 18n + 4p + 18in + 6ip + 18np + 9n^2 - 9p^2 + 5)/4$; $b_{16} = M - b_{15} - ea_{4i}$
G_2/A_{5i}:$1 \leq i \leq (n - p + 1)/2$; $ea_{5i} = 3p + 3i - 3$
$a_{17} = 3p^2 + (2i - 1)(6p + 3i - 3)$; $a_{18} = N - a_{17}$ $b_{17} = (18i^2 + 36ip - 36i + 9p^2 - 25p + 16)/2$; $b_{18} = M - b_{17} - ea_{5i}$
G_2/A_{6i}: $1 \leq i \leq (n - p - 1)/2$; $ea_{6i} = 3p + 3i - 1$
$a_{19} = 3p^2 + 12pi + 3i(2i - 1)$; $a_{20} = N - a_{19}$ $b_{19} = (18i^2 + 36ip - 18i + 9p^2 - 7p + 2)/2$; $b_{20} = M - b_{19} - ea_{6i}$
G_2/A_{7i}: $1 \leq i \leq p$; $ea_{7i} = 3i - 1$
$a_{21} = 3i^2$; $a_{22} = N - a_{21}$ $b_{21} = (9i^2 - 7i + 2)/2$; $b_{22} = M - b_{21} - ea_{7i}$

Following the computational procedure adopted in [5, 26] , we present the values of various distance-based topological indices of $HBC(p, q, n)$, for the case $p < q < n$, $q - p$ odd and $n - p$ odd.

□

4 Conclusion

Understanding the extensive use of polycyclic aromatics in industries like pharmaceuticals, chemicals, petroleum and their chemical and biological behaviours is crucial. These molecules are gaining traction due to their potential as semiconducting materials in devices like organic field-effect transistors, light-emitting diodes and solar panels. Employing methods like QSAR and QSPR allows us to forecast many of these compounds' properties and potential hazards based on their molecular structures. By determining topological indices, we can gain insights into the physicochemical properties of PAHs. The molecular descriptors derived from these indices provide a comprehensive view of the compound's structural attributes. This understanding is not just crucial for material science but also offers valuable insights for drug discovery, predictive toxicology, and even astrochemistry. The data in this article can streamline lab processes, especially when examining the physicochemical attributes of bitrapezium-shaped HBC.

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