

Topological descriptors calculations for A_4 (He, C)

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Abstract

The sporadic Held group hides a concealed geometric superstructure within its algebraic essence. The model is realized as the uniform A_4 -graph, facilitating the assessment of a wide variety of molecular descriptor and the corresponding wiener distance-enumerating polynomial and topological generating polynomial. The overall consequence presents encapsulated formulations that analytically link the topological descriptors to two major elements: conjugacy class cardinalities and graph disc dynamics. This suggests that the intricate topology of the entire system is, in fact, a concealed expression of its fundamental algebraic base.

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1. Introduction

A topological index is an integer obtained from a structure that captures the core geometry of a molecule. The correlation to material attributes originates from an algebraic factor associated with the chemical component. Choosing a topological index fails to be arbitrary; it follows the strategic framework of structural information classification (SIC). Geodesic-structural indices (GSI) are given more weight if the property of interest is affected by molecule shape. If the local bonding environment is important, valency-structural indices (VSI) are used. When it comes to qualities that have to do with molecular compactness or centrality, center-structural indices (CSI) are important. This methodology changes how descriptor selection is done from estimating to developing theories,

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see [1-11]. Prominent instances in the literature refer to the computation of topological descriptors for subdivision graphs and a comprehensive investigation of the Wiener index for several signed graphs. Topological indices, produced by graphs defined by group-theoretic interactions among vertices and edges, determine distinct geometric attributes within an inherently algebraic framework. Many recent studies have focused on topological descriptors for graphs based on group elements. Significant studies include those referenced in [12-18]. For example, a variety of topological indices have been computed for non-commuting graphs arising from finite non-abelian groups, as well as for order divisor graphs of cyclic groups. The A_4 -graph, expressed by the symbol, $A_4(G, C)$, is a discrete invariant with vertex set C – class of G . The adjacency condition yields that $\omega, \varsigma \in C$ produce an edge within $A_4(G, C)$, whenever $\langle \omega, \varsigma \rangle$ equal to the A_4 -group. To acquire knowledge more about this graph, examine out [19-20]. It is worth noting that reference [20] includes a structural analysis of the (He, C) . In that work, investigators passed an important target by meticulously describing the complex structure of the A_4 -graph for the primary conditions under which C is categorized as type $3A$ or $3B$. This study aims to create succinct guidelines that mathematically link the connectivity indicators of this graph into two main components. The capacity of the orbits (under the conjugation action) and the range of the graphical disk. The specific phrases for graph invariants utilized during this article are identical as those defined in references [17], [21].

2. SIC of $A_4(He, C)$

Let $\vartheta(C) = A_4(He, C)$, our objectives are mainly two-fold: (i) to compute the (SIC) descriptors for this graph, and (ii) to examine its metric topology. We define the q^{th} – disc, $\varphi_q(\omega)$, for $q \in \mathbb{Z}^+$ and a point ω , as the set $\{\tau \in V(\vartheta(C)) : d(\omega, \tau) = q\}$. This section of the article will recognize and describe the unique qualities that control the behavior of these discs in the graph $\vartheta(C)$.

Lemma 1: [20] *For any point $\omega \in C$, $\vartheta(C)$ involves an individual component, with the arrangement of the discs on this component stated as below.*

- 1- *If $C = 3A$, then $\vartheta(C)$ contains 3^{th} – disc through a way that, $|\varphi_1(\omega)| = 756$, $|\varphi_2(\omega)| = 157932$, $|\varphi_3(\omega)| = 374431$.*
- 2- *If $C = 3B$, then $\vartheta(C)$ contains 4^{th} – disc through a way that, $|\varphi_1(\omega)| = 405$, $|\varphi_2(\omega)| = 117282$, $|\varphi_3(\omega)| = 7719456$, $|\varphi_4(\omega)| = 159656$.*

By the vertex transitivity property of $\vartheta(C)$, and since $\binom{|V|}{2} - |E(\vartheta(C))| = |E(\vartheta(C))^c|$. The upcoming corollary is an outgrowth of Lemma 1.

Corollary 2: *When $C = 3A, (3B)$ and $\omega \in V(\vartheta(C))$, $j = 3$ we possess $e(\omega) = j, (j + 1)$ and $deg(\omega) = 756, (405)$.*

Moreover, $SD(\omega) = \sum_{q=1}^{j,(j+1)} q \cdot \varphi_q(\omega)$ is the sum of geodesic for ω . Consequently, by compounding the aforementioned data, we gain, $|V(\vartheta(3A))| = 533120$, $|V(\vartheta(3B))| = 7996800$. Also, $|E(\vartheta(3A))| = 201,518,160$, $|E(\vartheta(3AB))| = 1,619,352,000$.

Furthermore, $|E(\vartheta(3A))^c| = 142,106,086,240$, $|E(\vartheta(3B))^c| = 31,934,185,848,000$.

2.1 VSI for $\vartheta(C)$

As established in Corollary 2, and given that the graph $\vartheta(C)$ is vertex-transitive, hence, $|\varphi_1(\omega)| = \deg(\omega)$ for all $\omega \in V(\vartheta(C))$. Accordingly, the first Zagreb index of $\vartheta(3A)$ can be derived as:

$$\begin{aligned} M_1(\vartheta(3A)) &= \sum_{\omega \in V(\vartheta(3A))} \deg(\omega)^2 = \sum_{i=1}^{|3A|} |\varphi_1(\omega)|^2 = |V(\vartheta(3A))| * |\varphi_1(\omega)|^2 \\ &= (533120756)^2 * 756 = 304,697,272,320 \end{aligned} \quad (1)$$

Following the method used to get (1) and employing the GAP system [21], we calculate the VSI scores for $\vartheta(C)$, as listed in Table 1.

Table 1
VSI values for $\vartheta(C)$

VSI of $\vartheta(C)$	$C = 3A$	$C = 3B$
$M_1(\vartheta(C)) = \sum_{\omega \in V(\vartheta(C))} \deg(\omega)^2$	304, 697, 272, 320	1, 311, 702, 720, 000
$M_2(\vartheta(C)) = \sum_{\zeta \omega \in E(\vartheta(C))} \deg(\omega) \deg(\zeta)$	115, 243, 656, 537, 600	265, 614, 211, 800, 000
$F(\vartheta(C)) = \sum_{\omega \in V(\vartheta(C))} \deg(\omega)^3$	230, 163, 878, 809, 920	531, 321, 397, 600, 000
$\bar{M}_1(\vartheta(C)) = \sum_{\zeta \omega \notin E(\vartheta(C))} \deg(\omega) + \deg(\zeta)$	214, 760, 394, 415, 680	25, 867, 691, 536, 880, 000
$\bar{M}_2(\vartheta(C)) = \sum_{\zeta \omega \notin E(\vartheta(C))} \deg(\omega) \deg(\zeta)$	18, 241, 646, 983, 142, 400	5, 241, 852, 300, 172, 200, 000
$RM_2(\vartheta(C)) = \sum_{\zeta \omega \in E(\vartheta(C))} \deg(\omega) - 1][\deg(\zeta) - 1]$	114, 926, 239, 704, 000	264, 385, 837, 632, 000
$Nk(\vartheta(C)) = \prod_{\omega \in V(\vartheta(C))} \deg(\omega)^2$	403, 036, 320	3, 238, 704, 000
$\Pi_1(\vartheta(C)) = \prod_{\omega \in V(\vartheta(C))} \deg(\omega)^2$	304, 697, 272, 320	1, 311, 950, 041, 000
$\Pi_2(\vartheta(C)) = \prod_{\omega \zeta \in E(\vartheta(C))} \deg(\omega) \deg(\zeta)$	115, 243, 656, 537, 600	256, 614, 211, 800, 000
$R(\vartheta(C)) = \sum_{\zeta \omega \in E(\vartheta(C))} \frac{1}{\deg(\omega) \deg(\zeta)}$	352.645	9, 875
$RR(\vartheta(C)) = \sum_{\zeta \omega \in E(\vartheta(C))} \sqrt{\deg(\omega) \deg(\zeta)}$	152, 348, 723, 0	655, 837, 560, 000

Contd....

$ABC(\vartheta(C)) = \sum_{\zeta\omega \in E(\vartheta(C))} \sqrt{\frac{\deg(\omega) + \deg(\zeta) - 2}{\deg(\omega)\deg(\zeta)}}$	10, 360, 468.42	113, 608, 875
$H(\vartheta(C)) = \sum_{\zeta\omega \in E(\vartheta(C))} \frac{2}{\deg(\omega) + \deg(\zeta)}$	266, 520	3, 998, 400
$SCI(\vartheta(C)) = \sum_{\zeta\omega \in E(\vartheta(C))} \frac{1}{\sqrt{\deg(\omega) + \deg(\zeta)}}$	5, 167, 128, 205	56, 900, 000

Computational connection links the initial disc of $\vartheta(C)$ to the indices in Table 1. Moreover, the ordered arrangement of the group He enforces an organized framework on $\vartheta(3A)$ and $\vartheta(3B)$; it is this latent structural knowledge that facilitates a substantially quicker calculation.

2.2 GSI for $\vartheta(C)$

By the transitivity property of the vertices in $\vartheta(3A)$, it follows that for all $\omega, \zeta \in V(\vartheta(3A))$ and each $m = 1, 2, 3$, we have $|\varphi_m(\omega)| = |\varphi_m(\zeta)|$. Moreover, since the distance between any two vertices are symmetric, thus

$$\begin{aligned}
 W(\vartheta(C)) &= \sum_{\{\omega, \zeta\} \subseteq 3A} d(\omega, \zeta) = \frac{1}{2} \sum_{\omega \in V(\vartheta(3A))} SD(\omega) = \\
 &= \frac{|3A|}{2} (|\varphi_1(\omega)| \cdot 1 + |\varphi_2(\omega)| \cdot 2 + |\varphi_3(\omega)| \cdot 3) \\
 &= 266560(756 + 315,864 + 1,123,293) = 479784809280 \quad (2)
 \end{aligned}$$

Now, the same producers could apply to get the GSI scores for the graph $\vartheta(C)$ as listed in Table 2 below:

Table 2
GSI values for $\vartheta(C)$

GSI of $\vartheta(C)$	$C = 3A$	$C = 3B$
$W(\vartheta(C)) = \sum_{\{\omega, \zeta\} \subseteq V(\vartheta(C))} d(\omega, \zeta)$	479784809280	96,112,425, 142,400
$Wp(\vartheta(C)) = d((\vartheta(C)), 3)$	59,134,636,692	61,688,836,6 08,000
$TW(\vartheta(C)) = \sum_{\{\omega, \zeta\} \subseteq V(\vartheta(C))} d(\omega, \zeta)$	0	0
$Hold(\vartheta(C)) = \sum_{\{\omega, \zeta\} \subseteq V(\vartheta(C))} \frac{1}{d(\omega, \zeta)^2}$	21817648177.78	3588609112 00
$H(\vartheta(C)) = \sum_{\{\omega, \zeta\} \subseteq V(\vartheta(C))} \frac{1}{d(\omega, \zeta)}$	54520138773.33	106917764, 60800
$DD(\vartheta(C)) = \sum_{\omega \neq \zeta} (\deg(\omega) + \deg(\zeta)) d(\omega, \zeta)$	171,920,704,976,496	7782021703 80,28800
$Gut(\vartheta(C)) = \sum_{\omega \neq \zeta} \deg(\omega) \deg(\zeta) d(\omega, \zeta)$	219,368,781,739,054, 080	1574840201 78,22960000 0

Contd....

$H_A(\vartheta(C)) = \sum_{\omega \neq \varsigma} \frac{(\deg(\omega) + \deg(\varsigma))}{d(\omega, \varsigma)}$	82,510,095,864,009.6	8651545927 88,4800
$H_M(\vartheta(C)) = \sum_{\omega \neq \varsigma} \frac{(\deg(\omega) \deg(\varsigma))}{d(\omega, \varsigma)}$	31,173,029,684,316,9 53.6	1753725385 06,2400000

The placement of the disks in $\vartheta(C)$ leads to the forms shown in Table 2. The organized shape of the relevant distance matrix also helps in the calculations for the above formula.

2.3 CSI for $\vartheta(C)$

Following the technique stated in the preceding sections, the CSI scores corresponding to $\vartheta(C)$ are displayed in Table 3.

Table 3
CSI values for $\vartheta(C)$

CSI of $\vartheta(C)$	$C = 3A$	$C = 3B$
$\xi(\vartheta(C)) = \sum_{\omega \in V(\vartheta(C))} e(\omega)$	1,599,360	31987200
$E_1(\vartheta(C)) = \sum_{\omega \in V(\vartheta(C))} (e(\omega))^2$	17,059840	127948800
$E_2(\vartheta(C)) = \sum_{\varsigma \omega \in E(\vartheta(C))} e(\omega)e(\varsigma)$	1813663440	25909632000
$\xi^c(\vartheta(C)) = \sum_{\omega \in V(\vartheta(C))} e(\omega)\deg(\omega)$	535388	12954816000
$C^\xi(\vartheta(C)) = \sum_{\omega \in V(\vartheta(C))} \frac{\deg(\omega)}{e(\omega)}$	134,346,240	809676000
$\xi^d(\vartheta(C)) = \sum_{\omega \in V(\vartheta(C))} e(\omega)SD(\omega)$	2302939255680	768715142899200
$\xi^{sv}(\vartheta(C)) = \sum_{\omega \in V(\vartheta(C))} \frac{e(\omega)SD(\omega)}{\deg(\omega)}$	3045425469.5238	1898062081232593

Every record in **Table 3** is calculated according to **Corollary 1**, following the rules for getting GSI and VSI values.

Corollary 2:

1- The Wiener polynomial of $\vartheta(C)$ is expressed in relation to the variable u as follows:

$$WP(\vartheta(3A), u) = 533120 + 756u + 157932u^2 + 374431u^3, \text{ and}$$

$$WP(\vartheta(3B), u) = 7996800 + 405u + 117282u^2 + 7719456u^3 + 159656u^4.$$

2- The topological polynomial of $\vartheta(C)$ is $\{|\varphi_1(\omega)| * |C| | (WP(\vartheta(C), u) - |C|)\}$ for any point $\omega \in C$.

Proof: Consider $\tau \in V(\vartheta(C))$, then

$$WP(\vartheta(3A), u) = \sum_{\zeta=0}^3 d(\vartheta(3A), u)u^\zeta = 533120 + |\varphi_1(\tau)|u + |\varphi_2(\tau)|u^2 + |\varphi_3(\tau)|u^3 = 533120 + 756u + 157932u^2 + 374431u^3 \quad (3)$$

We attain through a similar strategy:

$$WP(\vartheta(3B), u) = 7996800 + 405u + 117282u^2 + 7719456u^3 + 159656u^4$$

For the next point,

$$\begin{aligned} TP(\vartheta(C), u) &= \sum_{\mu \neq \gamma \in C} (deg(\tau) + deg(\omega)) u^{d(\tau, \omega)} \\ &= 2 * |\varphi_1(\omega)| \sum_{C \neq k \in C} u^{d(\tau, \omega)} = 2 * |\varphi_1(\omega)| \frac{|C|}{2} (SD(\tau)) \\ &= |\varphi_1(\omega)| * |C| (WP(\vartheta(C), u) - |C|) \quad (4) \end{aligned}$$

3. Conclusion

The results above show that the algebraic components of the group He serve as an ideal framework for topological geometry. Using his A_4 -graph model, we obtain mathematical descriptors that correctly combine topological constants with the orbits sizes (under conjugation action) and disk growth dynamics. This indicates that the topological indicators of this graph are not only related to its algebraic base, but are also strongly influenced by the structure itself. Larger He -class size produce greater topological descriptors for the associated A_4 -graph.

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