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SOME NEW TOPOLOGICAL INDICES ON UNITARY CAYLEY QUOTIENT GRAPHS

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Abstract

Numerical metrics related to the fundamental attributes of a chart are referred to as topological lists. They play an essential role in theoretical chemistry, especially in simulating the chemical, natural, and physical properties of atoms.The Unitary Cayley Remainder Charts are a distinct set of logarithmic charts noted for their continuity defined by unit elements in Zn, created from the additive group of integrability modulo Zn. This series of charts is the focus of this examination. We derive explicit equations for the over topological lists and examine the fundamental features of these systems. The results demonstrate the symmetric and distance-regular properties of unitary remainder Cayley graphs and establish a foundation for further advancements in graph theory and computational chemistry. The ease of these charts in replicating atomic structures with standard removal conveyance is further demonstrated by our results.

Key Words and Phrases: Distance, Distance Matrix, Unitary Cayley Graph, Topological Index.

1. Introduction

Linking atomic structure to physical and chemical characteristics is one of the primary goals of theoretical chemistry. The Chemical Chart Hypothesis (CGT) stems from the substantial investments in this field over the past fifty years through graph-theoretical and information-theoretical methods. CGT examines the connections between structural properties and structural movements through the use of statistical techniques and graph theory.

The topological characterization of particles simplifies the classification and property prediction for obscure chemical structures. A crucial element of CGT is the inclusion of substance models, which separate atomic traits and reassemble their component values. Central to this effort are topological lists (TIs), which are numerical representations of graphs.

In QSAR and Quantitative Structure–Property Relationship (QSPR) studies, topological lists are frequently employed to estimate physical and chemical properties such as polarity,

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viscosity, melting point, and boiling point. The Wiener list, serving as the foundation for various similar lists, is the most widely recognized among the many records, approximately 400 that have been created. In this study, we create various relevant distance-based topological structures and examine a distinct category of graphs. Topological indices were studied in [2,3,4,5,6].

2. Definitions and Preliminary Results

Let $n > 1$ be an integer and $S = \{s : s\ ,\ is\ a\ unitary\ divisor\ of\ n\}$

Then the set $S^* = \{0,\ s,\ n - s\ : s \in S\}$ is the subset of Z_n then the graph associated with S^* is denoted as $G(V, E)$ with vertex set $V = Z_n$ and $E = \left\{u, v : either\ \frac{u}{v}\ or\ \frac{v}{u} \in S^*\right\}$ is termed as unitary Cayley quotient graph

Lemma: 2

The number of edges of unitary Cayley quotient graph $\tau(n)$ is

$$\tau(n) = \mathrm{n} + \varphi(n) - 2 + \sum_{1<k<\left[\frac{n}{2}\right]} \sum_{\substack{k<d<n \\ \frac{d}{k} \in S^*}} 1\ ,$$

where $\varphi(n)$ is the Euler totient function and $[x]$ is the greatest integer function.

Proof

It is clear that the number of units in the ring Z_n is ϕ(n), and the generating set S^* contains the element {0}, 0 can be expressed as product with any other number and $\frac{0}{a} = 0 \in S^*$. Therefore, the vertex 0 is adjacent with all other remaining vertices of the graph. Similarly, the vertex 1 is adjacent with every vertice v_i, i ∈ S. So for these two cases we obtained $n + ϕ(n) - 2$ edges, since 2 divides every even integer, hence the vertex 2 is adjacent with the vertices v_{2i}, i = 2, 3, … , $[^n]$ if and only if i ∈ S^* similarly the vertex v_3 adjacent with the vertices v_{3i}, i = 2, 3, … , $[^n]$ if and only if i ∈ S^* and so on. Summing all these values we get $\tau(n) = n + \varphi(n) - 2 + \sum_{1<k<\left[\frac{n}{2}\right]} \sum_{\substack{k<d<n \\ \frac{d}{k} \in S^*}} 1$Hence the result.

Theorem 5

The wiener index of unitary quotient cayley graph is

$$W(G) = (n-1)^2 - \varphi(n) + 1 - \alpha\ ,\quad for\ n \geq 2$$

Where $\alpha = \sum_{1<k<\left[\frac{n}{2}\right]} \sum_{\substack{k<d<n \\ \frac{d}{k} \in S^*}} 1$

Proof

Since G is the Unitary quotient Cayley graph of order n ≥ 2 with edges $\tau(n)$ Now the distance matrix is given by$D(G) = \left(d_{ij}\right)_{n\times n}$ and it is clear that,$\frac{i}{j} \in S^* or\ \frac{i}{j} \in S^*$,then the vertices v_i and v_j are adjacent, distance between them is 1, otherwise the distance between the vertices v_i and v_j is 2.

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Since $\frac{0}{i} = 0 \in S^* \; and \; \frac{0}{j} = 0 \in S^*$ and so is adjacent with the vertex 0 and is also adjacent with the vertex 0. Hence there exists a path $(v_i e_{i1} v_1 e_{ij} v_j)$ between the vertices v_i and v_j of length 2, therefore $d_{ij} = \begin{cases} 1 \; , \frac{i}{j} \in S^* or \; \frac{i}{j} \in S^*, \\ 2 \; , \frac{i}{j} \notin S^* or \; \frac{i}{j} \notin S^* \end{cases}$ Hence the element 1 occurring 2 $\tau(n)$ times and the element 2 occurring $2[nC_2 - \tau(n)\,]$ times in the distance matrix D(G). By the definition of wienerindex, we have

$$W(G) = \frac{1}{2} \sum_{v_i, v_j \in V(G)} d_{ij}$$

$$= \frac{1}{2}\{2\tau(\mathrm{n}) \times 1 + 2[nC_2 - \tau(n)\,] \times 2\}$$

$$= \tau(n) + 2 \times \left[\frac{n(n-1)}{2} - \tau(n)\right]$$

$$= n^2 - n - \tau(n)$$

$$= n^2 - n - (n + \varphi(n) - 2 + \sum_{1<k<\left[\frac{n}{2}\right]} \sum_{\substack{k<d<n \\ \frac{d}{k} \in S^*}} 1$$

$$= (n-1)^2 - \varphi(n) + \alpha$$

Where $\alpha = \sum_{1<k<\left[\frac{n}{2}\right]} \sum_{\substack{k<d<n \\ \frac{d}{k} \in S^*}} 1$. It completes the proof.

Theorem 6

The hyper wiener index of the Unitary quotient Cayley graph of order n ≥ 2 vertices and $\tau(n)$ edges is, $HW(G) = 3n^2 - 7n + 8 - 4(\alpha + \varphi(n))$

Proof

Here G is the Unitary quotient Cayley graph of order n ≥ 2 graph of order n ≥ 2

with edges $\tau(n)$. Let $v_1, \; v_2, \; \ldots \;, \; v_n$ be the vertices of G. For n ≥ 2, by the definition of hyperwiener index and using the distance matrix, we have

$$HW(G) = \frac{1}{2} \sum_{vi, vj \in G(V)} (dij + d^2 ij)$$

$$= \frac{1}{2} \sum_{v_i, v_j \in V(G)} {d_{ij}}^2 + \frac{1}{2} \sum_{v_i, v_j \in V(G)} d_{ij}$$

$$= \frac{1}{2} \sum_{v_i, v_j \in V(G)} {d_{ij}}^2 + W(G)$$

$$= (n-1)^2 - \varphi(n) + 1 - \alpha + \frac{1}{2}\{2\tau(\mathrm{n}) \times 1^2 + 2[nC_2 - \tau(n)\,] \times 2^2\}$$

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$$= (n-1)^2 - \varphi(n) + 1 - \alpha + \tau(\mathrm{n}) + 4\left[\frac{n(n-1)}{2} - \tau(n)\right]$$

$$= 3n^2 - 7n + 8 + 4(\alpha + \varphi(n))$$

Hence the proof.

Theorem 6

The Harary index of the Unitary quotient Cayley graph of order n ≥ 2 vertices and $\tau(n)$ edges is, $HI(G) = \frac{1}{4}(n^2 + n - 4 + 2(\alpha + \varphi(n))$

Proof

Here G is the Unitary quotient Cayley graph of order n ≥ 2 graph of order n ≥ 2 with edges $\tau(n)$. Let $v_1, v_2, \ldots, v_n$ be the vertices of G. For n ≥ 2, by the definition of Harary index and using the distance matrix, we have

$$HI(G) = \frac{1}{2}\sum_{vi,vi\in G(V)} \frac{1}{dij}$$

$$= \frac{1}{2}\left\{2\tau(\mathrm{n}) \times 1 + 2[nC_2 - \tau(n)\,] \times \frac{1}{2}\right\}$$

$$= \left\{\tau(\mathrm{n}) + [nC_2 - \tau(n)]\frac{1}{2}\right\}$$

$$= \frac{1}{4}(n^2 + n - 4 + 2(\alpha + \varphi(n))$$

This completes the proof.

Theorem 7

The Hyper Harary index of the Unitary quotient Cayley graph of order n ≥ 2 vertices and $\tau(n)$ edges is, $HHI(G) = \frac{1}{8}(3n^2 + 7n - 20 + 10(\alpha + \varphi(n))$

Proof

Here G is the Unitary quotient Cayley graph of order n ≥ 2 graph of order n ≥ 2 with edges $\tau(n)$. Let $v_1, v_2, \ldots, v_n$ be the vertices of G. For n ≥ 2, by the definition of Hyper Harary index and using the distance matrix, we have

$$HHI(G) = \frac{1}{2}\sum_{v_i,v_j\in V(G)} \frac{1}{d_{ij}} + \frac{1}{{d_{ij}}^2}$$

$$= \frac{1}{2}\sum_{v_i,v_j\in V(G)} \frac{1}{d_{ij}} + \frac{1}{2}\sum_{v_i,v_j\in V(G)} \frac{1}{{d_{ij}}^2}$$

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By solving the second summation will get the result. It completes the proof

3. Conclusion

The Wiener record, hyper Wiener list, Harary record, and hyper Harary file for Unitary Cayley Remainder Charts are four essential distance-based topological records for which we have obtained clear definitions in this paper. These graphs possess remarkable fundamental symmetries that simplify the computation of these records. They are defined by the additional substance group Zn with individual requirements on adjacency. The closed-form equations provided are crucial because they illuminate the inner remove dispersion of these charts and demonstrate their potential for modeling atomic structures in chemical chart theory. Our research encompasses the expanding literature on arithmetic and distance-oriented features of Cayley-type graphs from a mathematical perspective. When such charts are used to represent atomic systems, these files can be regarded as indicators of atomic properties from the standpoint of chemical modeling. Future research could explore dreadful lists, utilize these findings in weighted or combined versions of unitary Cayley diagrams, or integrate the resulting data into machine learning algorithms for cheminformatics property prediction. Furthermore, the practical centrality of the established graph-theoretical results can be further validated through comparisons with empirical chemical data.

References

[1] Sripaisan, Naparat, and YotsananMeemark. "Algebraic degree of spectra of Cayleyhypergraphs." *Discrete Applied Mathematics* 316 (2022): 87-94.

[2] Ramaswamy, H. N., and C. R. Veena. "On the energy of unitary Cayley graphs." *the electronic journal of combinatorics* (2009): N24-N24.

[3] Lin, Henry W. "Cayley graphs and complexity geometry." *Journal of High Energy Physics* 2019, no. 2 (2019): 1-15.

[4] R. Binthiya, Jisha J.J., T.M. Selvarajan. , Some Indices on Divisor Graph of First N Natural Numbers, Panamerican Mathematical Journal.2025, vol 35, No. 1,134-140.

[5] R. Binthiya, *Uma. M*, T.M. Selvarajan., Some Indices on Unitary Cayley Quotient Graph Panamerican Mathematical Journal.2025, vol 35, No. 1,141-146.

[6] Liu, Xiaogang, and Sanming Zhou. "Eigenvalues of Cayley graphs." *arXiv preprint arXiv:1809.09829* (2018).

[7] Cooperman, Gene, Larry Finkelstein, and NamitaSarawagi. "Applications of cayley graphs." In *International symposium on applied algebra, algebraic algorithms, and error-correcting codes*, pp. 367-378. Springer, Berlin, Heidelberg, 1990.

[8] Bojan mohar and Tom~ pisanski, How to compute the wiener index of a graph Journal of Mathematical Chemistry 2(1988)267 277

[9] Konstantin Vorob'ev Wiener index and graphs, almost half of whose vertices satisfy Soltes property

[10] Xiaohai Su · Ligong Wang · Yun Gao, Wiener Index of Graphs and Their Line Graphs JORC (2013) 1:393–403 DOI 10.1007/s40305-013-0027-6

[11] Gordon Cash, sandi Klavzar, Marko PetkovsekThree Methods for Calculation of the Hyper-Wiener Index of Molecular Graphs*J. Chem. Inf. Comput. Sci.* 2002, 42, 3, 571–576

[12] Istavan Lukovits, A note on a formula for the hyper-Wiener index of some trees

[13] DeDeo, M. R. "On the Energy of Transposition Graphs." In *Southeastern International Conference on Combinatorics, Graph Theory, and Computing*, pp. 305-316. Springer, Cham, 2022.

[14] ANUSHA, M. VENKATA, M. SIVA PARVATHI, K. MANJULA, and GS SHANMUGA PRIYA. "ENERGY OF EULER TOTIENT CAYLEY GRAPH." (2022).

[15] Lin, Henry W. "Cayley graphs and complexity geometry." *Journal of High Energy Physics* 2019, no. 2 (2019): 1-15.

[16] Akbari, Saieed, Amir HosseinGhodrati, Ivan Gutman, Mohammad Ali Hosseinzadeh, and Elena V. Konstantinova. "On path energy of graphs." *MATCH Commun. Math. Comput. Chem* 81, no. 2 (2019): 465-470.

[17] Philipose, Roshan Sara, and P. B. Sarasija. "Minimum Covering Gutman Energy of Unitary Cayley Graphs.