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Wiener Index Calculation on the Benzenoid System: A Review Article

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Abstract

The Weiner index is considered one of the basic descriptors of fixed interconnection networks because it provides the average distance between any two nodes of the network. Many methods have been used by researchers to calculate the value of the Wiener index. starting from the brute force method to the invention of an algorithm to calculate the Wiener index without calculating the distance matrix. The application of the Wiener index is found in the molecular structure of organic compounds, especially the benzenoid system. The value of the Wiener index of a molecule is closely related to its physical and chemical properties. This paper will show a comprehensive bibliometric survey of peer-reviewed articles referring to the Wiener index of benzenoid. The Wiener index values of several benzenoid compounds are also reported. The Wiener index of benzenoid supports much of the research and provides productive citations for citing the study.

Keywords: Wiener index, benzenoid, distance matrix, chemical properties, cubic polynomial, topological.

1. Introduction

In the last two decades, the development of information and communication technology has progressed very rapidly. This is due to the strong era of globalization, where computers and the internet are facilities that have dominated various activities of life, including office, commercial, and scientific research. This characteristic of society is known as a "knowledge-based society," meaning that a community that masters knowledge has the opportunity to utilize information and make information an added value in their lives. Someone often becomes the author of a scientific paper that contributes to scientific matters and makes frequent references to the bibliography. However, until now, the need for bibliometric studies has not been explored by many people. Bibliometric is a mapping analysis method of bibliographic information obtained from high-impact databases that can be applied in various fields of science (García-Corral *et al.*,[1]). Bibliometrics has been widely used in science policy and research

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management for decades. The study of bibliometrics can be applied in various fields such as education, management, science, economics, and marketing.

Mathematics is a rich and complex science, a basic science as well as a tool for solving problems that arise in other sciences. For example, they were estimating income or the curve of fluctuations in income with the theory of Black-Scholes. In biology, genotypes can be determined that are superior to plant breeds. In physics, the effects of a force on an object are determined, whereas in computer programs, an error value is generated using Python's script. In chemistry, one of the interesting branches of mathematical chemistry to study is *chemical graph theory*. Chemical graph theory is a branch of mathematics that associates graph theory with chemistry (Zhao *et al.*, [2]). The chemical graph theory is a branch of graph theory that deals with the mathematical modeling of molecules (Turaci, [3]). It is a branch of graph theory that applies to chemistry and focuses on the concept of a chemical graph (Gracía-Fomenech *et al.*, [4]). It is also considered a fascinating branch of graph theory, which has many applications related to chemistry, drug designs, etc. Graph theory was first introduced by Leonhard Euler in 1736. Euler's solution to the Konigsberg bridge problem, in the form of nodes and edges, was a precursor to the development of the concept of a graph. Since then, graphs have been widely used in many areas such as chemistry, biology, and social network analysis (Hassan *et al.*, [5]).

In general, a graph is used to represent a molecule by considering the atoms as the vertices of the graph and the molecular bonds as the edges (Estrada and Bonchev, [6]). A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. The vertices in G are connected by an edge if there exists an edge $uv \in E(G)$ connecting the vertices u and v in G such that $u, v \in V(G)$. The number of vertices and edges in a graph will be denoted by $|V(G)|$ and $|E(G)|$, respectively. The molecular graph is related to topological indices; therefore, chemical compound properties like, fracture toughness, boiling point, rigidity, and strain energy can be evaluated by these indices (Zuo *et al.*, [7]). A numerical value that represents the topology of a graph is known as the topological index. A topological or molecular descriptor or index is a topologically invariant mathematical real number defined for a finite simple graph such that it has significant application in chemistry (Zhao, [2]). According to the IUPAC, "*a topological index* (or *molecular structure descriptor*) is a numerical value associated with the chemical constitution for the correlation of chemical structure with various physical properties, chemical reactivity, or biological activity." (Julietraja *et al.*, [8]).

Topological indices are very important for predicting the biological activities of chemical compounds, and they have a lot of applications in QSAR and QSPR (Alishahi and Shalmaee, [9]). The Wiener index is the oldest topological index related to molecular branching (Wei and Shiu, [10]). The Wiener index, defined as the sum of all distances between pairs of vertices in a graph, was probably the first and most studied such graph invariant, appearing in 1947 (Chen *et al.*, [11]). It is employed to predict the boiling points of alkane molecules (Harry, [12]), and it is also correlated with other quantities, including the parameters of its critical point (Stiel and Thodos, [13]). heats of vaporization, molar volumes, and molar refractions of alkanes (Manuel *et al.*, [14]). The Wiener index of a graph G is denoted by $W(G)$ and defined as the sum of distances between all pairs vertices in G (Chen *et al.*, [11]).

$$(G) = \sum_{u,v \subset V((G)} d_G(u, v) = \frac{1}{2} \sum_{v \in V(G)} D_G(v). \tag{1}$$

The vast majority of molecules of interest in chemistry, such as the benzenoid system, are cyclic. A benzenoid system is a finitely connected planar subgraph of an infinite hexagonal system, or a honeycomb lattice, with no cut vertices and all the interior faces being regular hexagons (Julietraja *et al.*, [15]). A benzenoid system is a connected geometric figure obtained by arranging congruent regular hexagons in a plane, so that two hexagons are either disjoint or have a common edge. This figure divides the plane into one infinite (external) region and a number of finite (internal) regions. All internal regions must be regular hexagons. Benzenoid graphs or graph representations of benzenoid hydrocarbons are defined as finitely connected

plane graphs with no cut vertices, in which all interior regions are mutually congruent regular hexagons. Benzenoids are important raw materials in the chemical industry and are utilized in the manufacturing of many common materials such as dyes and plastics (Julietraja *et al.*, [8]).

In this study, we survey the total number of papers in the database using Google Scholar regarding the Wiener index of benzenoid chain graphs. It can also be seen how the research cluster was built. The bibliographic mapping analysis is done, and we examine the Wiener index of benzenoid chain graph themes that researchers have directed. We also calculate the Wiener indices of several benzenoid compounds using the method appropriate for each compound. The purpose of conducting bibliometric analysis is to study various calculations of the Wiener index on the benzonoid system proposed by various researchers. In addition, it is also important to see how far research has progressed on the development of the Wiener index for the benzenoid system. Bibliometric analysis can also be used to see if there is a relationship between the Wiener index and the eigenvalues, physical properties, and chemical properties of benzenoid compounds. Therefore, in this paper, we will present various formulas for calculating the Wiener index of catacondensed and pericondensed benzenoid representative systems. Then we will also see whether there has been any study of the relationship between the Wiener index values and the eigenvalues, bearing in mind that the eigenvalues of the benzenoid system can represent the physical and chemical properties of each benzenoid compound.

2. Method

2.1. **Data Collection.** In this study, the data taken was Scopus-indexed international publication data. collecting data through searching with the keywords "Wiener index" and "benzenoid." Search engines do this by searching for these keywords and returning a series of citations by year, rank, author, year, publications, publisher, and type. All papers received are from the Scopus database and science direct via Publish or Perish, as the data source is one of the most comprehensive peer-reviewed journal databases in the world and can provide good scientific and academic information. However, the maximum number of searches is limited to 1,000. The search results obtained are "Wiener index" and "benzenoid," with 1000 papers each. Keyword search applies only to titles and summaries. Kemudian big data tersebut disimpan dalam format Research Information System (RIS) format for bibliographic citations stored in RIS files.

2.2. **Bibliometric Analysis.** This bibliographic overview is a search for literature published on the Wiener Index of Benzenoid (WIB) in peer-reviewed journals published in the international language (written in English). This survey focuses only on works published between 2010 and 2022, but do not rule out discussing other literature that is still appropriate from previous years. Google Scholar (GLS) with Publish or Perish software is designed for individual scholars to present and retrieve citations from various data sources (Crossref, Google Scholar, Scopus, Microsoft Academic, and Web of Science) in literature searches. Publish or Perish results can be saved in a variety of formats using a custom format reader. The author uses the VOSViewer application to help with bibliometric analysis by visualizing data. With VOSViewer, bibliometric chart maps are easier to interpret to view a relationship or network. VOSViewer is a computer program used to visualize bibliometric maps (Herawati *et al.*, [16]). The text-mining function can be used to visualize a network or correlation in an article excerpt (Herawati *et al.*, [16]). The stage for using the VOSViewer software is to select *create-read data from bibliographic database files-next-cooccurence keywords-next-finish.* The bibliometric analysis carried out focused on co-occurrence keywords regarding the development of the Wiener index research on the benzenoid system. Then another analysis, namely, is there any research that specifically discusses the relationship between the Wiener index and the eigenvalues of benzenoid compounds based on the problem formulation in the introduction? The keywords chosen are related to the Wiener index research on the benzenoid system.

3. Result and Discussion

This chapter will discuss and elaborate on the formulation of the problem in the introduction, namely looking at the development of research on the Wiener index in the benzenoid system, presenting the formula for calculating the Wiener index value in the benzenoid system, and seeing whether there is research that specifically examines the relationship between the Wiener index and eigenvalues.

3.1. **Bibliometric Analysis.**

3.1.1. *Research Publication Summary.* This session outlines the papers published in the Wiener Index of Benzenoid. The number of papers received is shown in Figure 1. The graph shows different publishing patterns from 2010–2022, showing that the Wiener Index of Benzenoid is still being used as research support. The number of papers published varies from year to year. The articles published are in various scientific fields such as chemistry, computer science, physics, astronomy, engineering, biochemistry, genetics, molecular biology, etc.

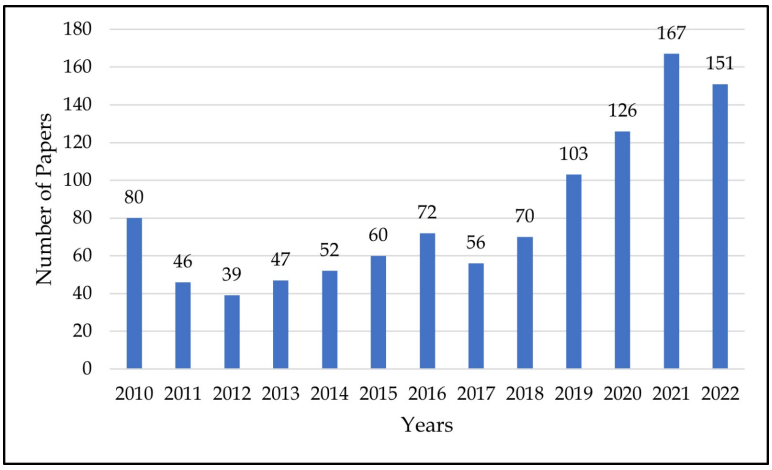

Figure 1. Number of publication of WIB per year.

In Figure 1, it can be seen that the researchers' interest in the Wiener index of benzenoid increased exponentially from 2011 to 2022. The majority of research was conducted in 2021, with 167 papers published. The least amount of research occurred in 2012, namely 39 papers.

Table 1. Top subject area that related to WIB.

Subject area	**Papers**
Mathematics	570
Chemistry	461
Computer science	197
Materials science	173
Physics and astronomy	137
Engineering	118
Biochemistry, genetics, and molecular biology	51
Chemical engineering	33
Pharmacology, toxicology and pharmaceutics	33
Multidisciplinary	22

Based on Table 1, it can be seen that the three largest subject areas of the Wiener index of benzenoid research during the 2010–2022 period were namely mathematics (31.75% or

570 documents), chemistry (25.68% or 461 documents), and computer science (10.97% or 197 documents).

Table 2. Top journals that publish WIB.

Journal title	**Papers**
Match	102
Polycyclic aromatic compounds	47
Journal of discrete mathematical sciences and cryptography	40
Journal of computational and theoretical nanoscience	36
Applied mathematics and computation	34
Journal of mathematical chemistry	32
Optoelectronics and advanced materials rapid communications	30

Table 2 shows that there are 10 journals with the highest productivity during 2011–2022 in the Wiener index of benzoid research. The top three positions are held by Match with 102 papers, 47 papers on polycyclic aromatic compounds, and 40 papers in the journal of discrete mathematical sciences and cryptography.

Table 3. Top country that publish papers related to WIB.

Country	**Papers**
China	321
Pakistan	245
Iran	214
India	155
Slovenia	85
United States	72
South Korea	47
Saudi Arabia	46
United Arab Emirates	44
Turkey	42

In Table 3, the contributors to the results of the Wiener index of benzenoid system research can be identified; the authors of the WIB articles are scattered in various countries. The countries that issued the most WIB articles were China with 321 articles, Pakistan with 245 articles, and Iran with 214 articles.

3.1.2. *Main Research Topic.* In the discussion of this section with the theme "Wiener Index of Benzenoid," by using software that can visualize bibliometric networks. The data that takes center stage in bibliometric analysis tends to be massive and objective in nature (number of citations and publications, occurrences of keywords, and topics), though its interpretations often rely on both objective and subjective evaluations established through informed techniques and procedures (Donthu *et al.*, [20]). In this study, we used VOSviewer software as a tool to perform the co-occurrence keywords analysis, and then to visualize the intellectual structure.

It can be seen in Figure 2 that the co-occurrence keywords network mentions WIB literature and identifies the clusters in different colors. For example, for each cluster, the keyword correlation shows the co-occurrence of the research network that has been conducted. The higher co-occurrence among networks indicates that extensive research has been conducted. On the contrary, if a little connectedness in the network shows that research with these keywords is an opportunity to become a prospective research topic, as seen in cluster 1 (red), graph theory, the Wiener index, and molecular structure have a large co-occurrence network, while the keywords in the benzenoid system have a small co-occurrence network. It can be used as a reference or as a prospective research theme. Whereas in cluster 2 (green), the topological

index has many co-occurrence networks, on the other hand, the line graph and atom-bond connectivity indices have a small number. In cluster 3 (blue), distance and molecular descriptors have many co-occurrence networks, behind the number of benzenoid hydrocarbons. In cluster 4 (yellow), the molecular graph keyword has many co-occurrence networks, but QSQR and physical chemistry have a small number. The relationship between clusters allows it to be used as a reference for prospective research.

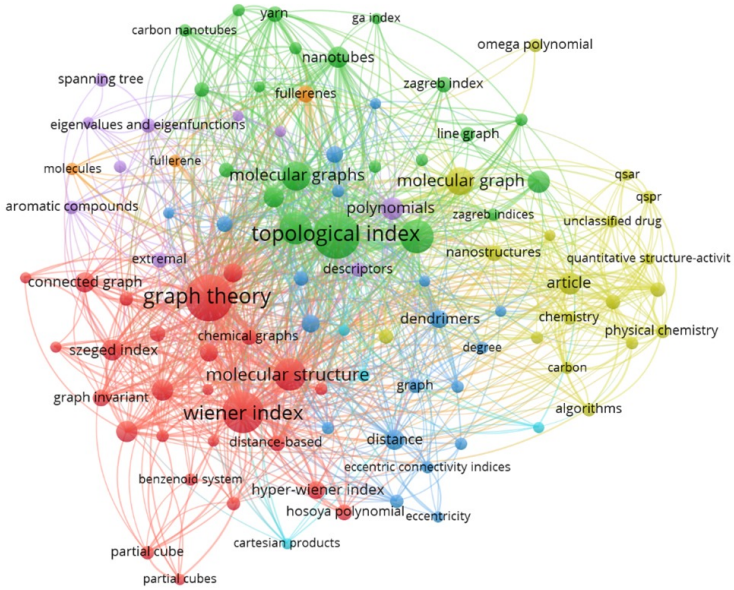

FIGURE 2. Bibliographic mapping of WIB research.

It can be seen that in the network visualization, each color represents one cluster. Each cluster is grouped in an interrelated circle among items and with other items in other clusters. In the bibliographic mapping of WIB research, there are 101 terms with the most occurrences being topological index (177), graph theory (166), Wiener index (135), and molecular structure (79), and there are keywords shown in Table 4.

Table 4: Popular keywords in each cluster of WIB research.

Cluster 1	**Cluster 2**	**Cluster 3**	**Cluster 4**
benzenoid system	atom-bond connectivity index	benzenoid hydrocarbons	algorithm
chemical graphs	atom-bond connectivity indices	boiling point	algorithms
connected graph	carbon nanotubes	computational chemistry	article
cut method	chemical graph theory	degree	carbon
distance-based	connectivity indices	dendrimer	chemical structure
extremal graph	ga index	dendrimers	chemistry
forestry	geometric-arithmetic index	diameter	molecular descriptor

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Table 4: Popular keywords in each cluster of WIB research. (Continued)

Cluster 1	**Cluster 2**	**Cluster 3**	**Cluster 4**
benzenoid system	atom-bond connectivity index	benzenoid hydrocarbons	algorithm
geometry	harmonic index	distance	molecular graph
graph g	line graph	eccentric connectivity index	mostar index
graph invariant	m-polynomial	eccentric connectivity indices	nanocone
graph theory	molecular graphs	eccentricity	nanostructures
graphic methods	nanotube	graph	omega polynomial
hosoya polinomials	nanotubes	mathematical chemistry	physical chemistry
hyper-wiener index	randic index	molecular descriptors	qsar
molecular structure	topological index	molecular graphics	qspr
partial cube	topological indices	nanostar	quantitative structure activity relation
pi index	topology	physicochemical properties	quantitative structure activity relationship
revised szeged index	vertex degree	polycyclic aromatic hydrocarbons	unclassified drug
sum of distances	yarn	topological descriptors	
szeged index	zagreb index		
tree	zagreb indices		
trees (mathematics)			
unicyclic graph			
wiener index			
wiener polarity index			

Cluster 5	**Cluster 6**	**Cluster 7**
aromatic compounds	cartesian products	fullerence
carbon nanocones	chemical compounds	fullerences
chains	degree-based index	molecules
descriptors	graph structures	
eigenvalues and eigenfunctions		
expected values		
extremal		
polynomials		
spanning tree		
theoretical chemistry		

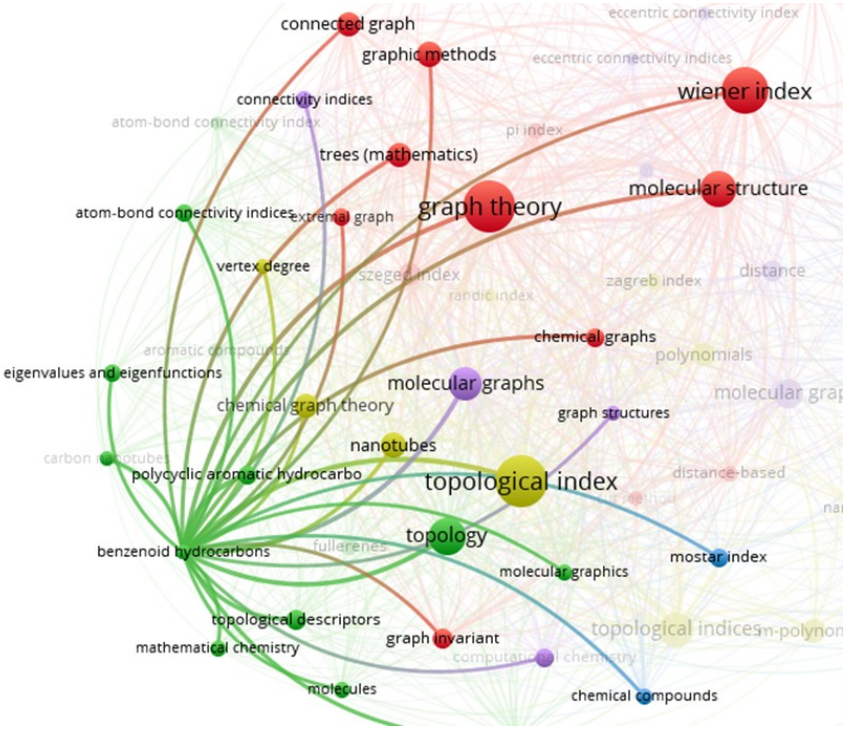

FIGURE 3. Bibliometric mapping of benzenoid hydrocarbons.

3.1.3. *The State of the Art on the Wiener Index of Benzenoid.* As mentioned in Figure 3, studies on the Wiener index and other related indices have indeed increased in recent years. However, studies on index topology, especially the Wiener index on benzenoid systems, are still few. In Figure 3, it can be seen that there are very few studies on benzenoid dengan occurrence 11 of 258. This is certainly a huge opportunity for researchers, especially in the field of mathematical chemistry. In Table 5, the author tries to present several studies on the Wiener index for benzenoid or related compounds. The articles in Table 5 below were selected based on research in this paper, namely the Wiener index, which focuses only on the benzenoid system. Most of them are the latest articles in the last 10 years, as well as articles that provide a fairly accurate method for calculating the Wiener index results in benzenoid systems.

Table 5: The state of the art on the Wiener index of benzenoid.

Writer	**Molecular Srtucture/ graph**	**Method**	**Focus of interest**	**Explanation**	**Result**
[38]	Benzenoid systems	Cut method	q, n_i, n	• q =length of benzenoid • n_i =number of vertices • $n = \|V(G)\|$ vertices	(2)
[39]	Naphthalene and trapezium benzenoid	Isometric Embedding method	n, k	• n= number of hexagon columns • k= number of hexagon rows	(3)

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Table 5: The state of the art on the Wiener index of benzenoid. (Continued)

Writer	**Molecular Srtucture/ graph**	**Method**	**Focus of interest**	**Explanation**	**Result**
[38]	Benzenoid systems	Cut method	q, n_i, n	• q =length of benzenoid • n_i =number of vertices • $n = \|V(G)\|$ vertices	(2)
[40]	Sodium chloride and honeycomb mesh (benzenoid)	Embedding and I-*Partition* method	m, n, k, d	• m, n, k = vertices number of three dimensional mesh • d = dimension of honeycomb mesh	(4)-(5)
[14]	C_4C_8 (S) Nanosheet, H-Naphtalenic Nanosheet, and Pericondenced benzenoid graphs	Embedding and *Partition* method	p, q, n, m, r, l	• p = columns number of C_4C_8 Nanosheet • q = rows number of C_4C_8 Nanosheet • n = columns number of Naphtalenic Nanosheet • m = rows number of Naphtalenic Nanosheet • r = vertical rows number of pericondensed benzenoid • l = horizontal graph number of pericondensed benzenoid	(6)-(11)
[10]	Polygonal chains	Recurrence method	k, n	• n = length of polygonal chains • k = possible ways to add bridge between cycles of polygonal chains	(12)-(16)
[27]	Polyomino chains	Edge cut method (I-*Partition* method)	s, p	• s = the number of segment in polyomino chains • p = the vertical cuts along the vertical segment	(17)-(23)
[35]	Daisy cubes	Isometric Embedding method	E_i	• E_i = the set of edges using the direction i.	(24)

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Table 5: The state of the art on the Wiener index of benzenoid. (Continued)

Writer	**Molecular Srtucture/ graph**	**Method**	**Focus of interest**	**Explanation**	**Result**
[38]	Benzenoid systems	Cut method	q, n_i, n	• q =length of benzenoid • n_i =number of vertices • $n = \|V(G)\|$ vertices	(2)
[41]	Polyacenes and Benzenoid system	Distance matrix and cubic polynomial	h	• h = variable of cubic polynomial (the number of cyclic hexagonals)	(25)-(34)

Equation (2)-(34) is a formula for calculating the Wiener index value of each benzenoid system obtained by the authors in Table 5. Table 6 contains detailed equations from (2) to (34).

Table 6: The state of the art on the Wiener index of benzenoid.

Equation Number	**Result**
(2)	$W(G) = \sum_{i=1}^{q} n_i(n - n_i)$
(3)	$W\left(T\left(n,k\right)\right) = \frac{4n^3\left(k^2+2k+1\right)}{3} - \frac{2n^2\left(k+1\right)\left(2k^2-8k-3\right)}{3} + \frac{2n\left(k^4-4k^3+6k^2+9k+1\right)}{3} - \frac{k\left(8k^4+35k^2-45k-28\right)}{30}$
(4)	$WI\left(M\left(m,n,k\right)\right) = \frac{mnk}{6}\left[nk\left(m^2-1\right)+mn\left(k^2-1\right)\right]$
(5)	$WI\left(G\right) = 6\left[\sum_{i=1}^{d-1}\mu_i\left(6d^2-\mu_i\right)\right] + 3\mu_0^2$
(6)	$W\left(T^1\left[2p,\ 2q\right]\right) = \frac{1}{6}q^2\left(p-q\right)\left(4p^2-2q^2+4pq+3p-3q-1\right)$
(7)	$W\left(T^2\left[2p,\ 2q\right]\right) = p^3\left(8q^2+\frac{40}{3}q+\frac{8}{3}\right) + p^2\left(\frac{8}{3}q^3+28q^2+\frac{112}{3}q+8\right) + p\left(\frac{8}{3}q^4+\frac{76}{3}q^2+\frac{104}{3}q+\frac{16}{3}\right) - \frac{8}{15}q^5+\frac{20}{3}q^4 - \frac{20}{3}q^3+\frac{16}{3}q^2+\frac{56}{5}q$

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Table 6: The state of the art on the Wiener index of benzenoid. (Continued)

Equation Number	**Result**
(8)	$W(G) = \frac{25}{3}nm(2m+n)(2nm-1) + 4\sum_{j=1}^{m} + \left((4k-1)+2\lfloor\frac{k-1}{2}\rfloor\right) \times \left(10nm - \sum_{i=1}^{j}\left((4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor\right)\right) + 2\sum_{j=1}^{2n-m-1}\left(\sum_{k=1}^{m}\left((4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor\right)\right) + j\left(4m+2+2\left\lfloor\frac{m-1}{2}\right\rfloor\right) \times \left(10nm - \left(\sum_{k=1}^{m}\left((4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor\right)\right. \right. + j\left.\left.\left(4m+2+2\left\lfloor\frac{m-1}{2}\right\rfloor\right)\right)\right)$
(9)	$W(G) = \frac{25}{3}nm(2m+n)(2nm-1) + 4\sum_{j=1}^{m}\left((4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor\right) \times \left(10nm - \sum_{i=1}^{j}\left((4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor\right)\right) + 2\sum_{j=1}^{2n-m-1}\left(\sum_{k=1}^{m}\left((4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor\right)\right) + j\left(4m+2\left\lfloor\frac{m-1}{2}\right\rfloor+j-\text{`}\right) \times \left(10nm - \sum_{k=1}^{m}\left((4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor\right)\right. + j\left.\left(4m+2\left\lfloor\frac{m-1}{2}\right\rfloor+j-1\right)\right)$
(10)	$W(G) = \frac{25}{3}nm(2m+n)(2nm-1) + 4\sum_{j=1}^{m}\left((4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor\right) \times \left(10nm - \sum_{i=1}^{j}\left((4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor\right)\right) + 2\sum_{j=1}^{2n-m-1}\left(\sum_{k=1}^{m}\left((4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor\right)\right) + j\left(4m+2\left\lfloor\frac{m-1}{2}\right\rfloor+j-\text{`}\right) \times \left(10nm - \sum_{k=1}^{m}\left((4k-1)+2\left\lfloor\frac{k-1}{2}\right\rfloor\right)\right. + j\left.\left(4m+2\left\lfloor\frac{m-1}{2}\right\rfloor+j-1\right)\right)$
(11)	$W(G) = \frac{r}{15}\left[-8r^4 + 20(2l+1)r^3 + 10\left(8l^2+8l+3\right)r^2 + 10\left(8l^3+12l^2+3l-2\right)r - 20l^2 - 20l - 7\right]$
(12)	$W(PC_n) = W(PC_{n-1}) + 2kd(v_{n-1}\|PC_{n-1}) + k^3(2n-1) + 4k^4(n-1)$
(13)	$W(PC_n) = W(PC_{n-1}) + (2k+1)d(v_{n-1}\|PC_{n-1}) + \left(2k^3+7k^2+5k+1\right)(n-1) + k^3 + \frac{3k^2-k}{2}$

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Table 6: The state of the art on the Wiener index of benzenoid. (Continued)

Equation Number	**Result**
(14)	$W\left(PC\left(n;p_1,p_2,\ldots,p_k\right)\right)=\left(\frac{2k^2}{3}\sum_{j=1}^{k}\left(j+1\right)p_j\right)n^3+2k^2\left(k+1-\sum_{j=1}^{k}(j+1)p_j\right)n^2+k^2\left(\frac{4}{3}\sum_{j=1}^{k}\left(j+1\right)p_j-k-2\right)n$
(15)	$W\left(PC\left(n;p_1,p_2,\ldots,p_k\right)\right)=\frac{(2k+1)^2}{6}\sum_{-=1}^{k}\left[(i+1)p_i\right]n^3+\left\{2k^3+5k^2+3k+\frac{1}{2}-\frac{(2k+1)^2}{2}\sum_{i=1}^{k}\left[(i+1)p_i\right]\right\}n^2+\left\{\frac{(2k+1)^2}{3}\sum_{i=1}^{k}\left[(i+1)p_i\right]-\left(k^3+\frac{7}{2}k^2+\frac{5}{2}k+\frac{1}{2}\right)\right\}n$
(16)	$W\left(\mathcal{PC}_n\right)=\frac{1}{\left\|\mathcal{PC}_n\right\|}\sum_{G\epsilon\mathcal{PC}_n}W\left(G\right)$
(17)	$W\left(G_1\right)=\left(n+1\right)^2+\sum_{p-1}^{n}4p\left(n-p+1\right)$
(18)	$W\left(G_2\right)=8\left(s+1\right)+\sum_{p=1}^{\frac{s-1}{2}}\left(4p+1\right)\left(2s-4p+3\right)+\sum_{p=1}^{\frac{s+1}{2}}\left(4p-1\right)(2s-4p+5)$
(19)	$W\left(G_2\right)=8\left(s+1\right)+\sum_{p=1}^{\frac{s}{2}}\left[16p\left(s-2p+2\right)-2\right]$
(20)	$W\left(G_3\right)=8\left(2s+1\right)+\sum_{p=1}^{\frac{s}{2}}32\left[p\left(3s-6p+5\right)-\left(s-2p+2\right)\right]+\sum_{p=2}^{\frac{s+2}{2}}32(p-1)(s-2p+3)$
(21)	$W\left(G_3\right)=8\left(2s+1\right)+\sum_{p=1}^{\frac{s-1}{2}}32p(s-2p+1)+\sum_{p=1}^{\frac{s+1}{2}}32\left[\left(2p-1\right)\left(s-2p+2\right)+\sum_{p=2}^{\frac{s+1}{2}}\left(p-1\right)(s-2p+3)\right]$
(22)	$W\left(G_4\right)=8\left(3s+1\right)+\sum_{p=1}^{\frac{s}{2}}2\left[12p\left(12s-24p+19\right)-\left(66s-132p+119\right)\right]+\sum_{p=2}^{\frac{s+2}{2}}4\left[12p\left(6s-12p+7\right)-\left(39s-78p+11\right)\right]$

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Table 6: The state of the art on the Wiener index of benzenoid. (Continued)

Equation Number	**Result**
(23)	$W(G_4) = 8(2s+1) + \sum_{p=1}^{\frac{s-1}{2}}(12p-1)[6(s-2p)+5] + \sum + p = 1^{\frac{s+1}{2}}[36p(6s-12p+11) - (126s-252p+233)] + \sum_{p=1}^{\frac{s+1}{2}} 4[6p(6s-12p+17) - (39s-78p+111)]$
(24)	$W(G) = \lvert V(G)\rvert \cdot \lvert E(G)\rvert - \sum_{i=1}^{n} \lvert E_i\rvert^2$
(25)	$W(L_h) = (16h^3 + 36h^2 + 26h + 3)/3$, for linear polyacenes, $1 \leq h \leq 4$.
(26)	$W(A_h) = (16h^3 + 24h^2 + 62h - 21)/3$, for zig-zag polyacenes
(27)	$W(H_h) = (8h^3 + 72h^2 - 26h + 27)/3$, for helicenes
(28)	$W(B_h) = 4h^3 + 16h^2 + 8h - 3 + (-1)^h(2h-4)$, for another benzenoid, $h = 8$.
(29)	$W(C_h) = 4h^3 + 16h^2 + 4h + 5 - (-1)^h(2h-4)$, for another benzenoid, $h = 8$
(30)	$W(D_h) = (16h^3 + 24h^2 + 74h - 39)/3 - 2(-1)^h$, for another benzenoid, $h = 8$.
(31)	$W(E_h) = (16h^3 + 24h^2 + 74h - 51)/ + 6(-1)^h$, for another benzenoid, $h > 1$.
(32)	$W(F_h) = 4h^3 + 20h^2 - 8h + 13 - (-1)^h(2h-4)$, for another benzenoid, $h = 8$.
(33)	$W(J_h) = 4h^3 + 20h^2 - 12h + 21 + (-1)^h(2h-4)$, for another benzenoid, $h > 1$.
(34)	$W(K_h) = (16h^3 + 30h^2 - 38h)/3 + (-1)^h$, for another benzenoid, $h > 1$.

Equations (25) to (34) are equations that are specific to the benzenoid system, as presented in Figure 4.

Benzenoid hydrocarbons (the benzenoid system) possess intriguing (and somewhat mysterious) electronic properties and have been attracting the interest of theoretical chemists for well over 150 years. In addition, they are important raw materials for the chemical industry (used, for instance, for the production of dyes and plastics), but they are also dangerous pollutants. The benzenoid compounds studied by the match journal are mostly used in drug design in the pharmaceutical industry (Gutman and Polansky, [41]). The same research on several benzenoid compounds was also conducted by the journal Acta Applicandae Mathematicae (Dobrynin *et al.*, [42]). They attempted to summarize a set of polynomials that correspond to and fit the structure of benzenoid compounds. The methods they use are also efficient and not time-consuming. In the following, we try to calculate the Wiener index values of several benzenoid compounds using the methods from Gutman and Polansky, [41], and Dobrynin *et al.*, [42] (as seen in Table 7).

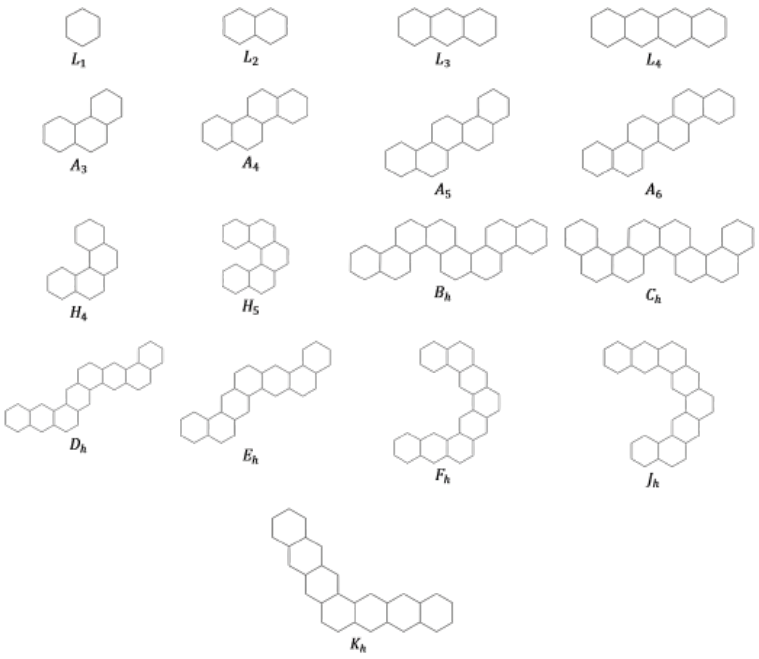
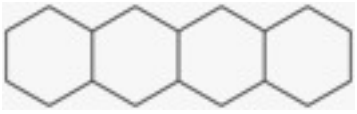


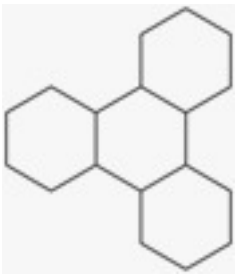
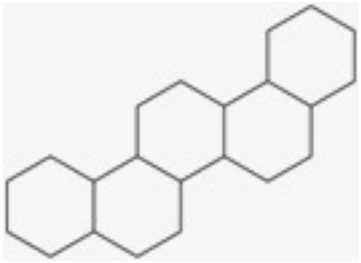
FIGURE 4. Benzenoid graph for equation (25)-(34).

Table 7: Wiener index values of several benzenoid system compounds.

Benzenoid Graph	**Compound Name**	**Wiener Index**
	naphthalene	109
	anthracene	279
	phenanthrene	271
	naphthacene	569

Continued on next page

Table 7: Wiener index values of several benzenoid system compounds. (Continued)

Benzenoid Graph	Compound Name	Wiener Index
	tetraphene	545
	chrysene	545
	triphenylene	535
	picene	963
	pentacene	1,011
	coronene	708.5

Continued on next page

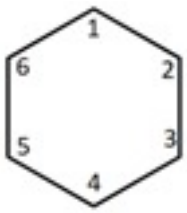
Table 7: Wiener index values of several benzenoid system compounds. (Continued)

Benzenoid Graph	Compound Name	Wiener Index
	heptacene	2,479
	octacene	3,569
	decacene	6,621

The calculation of the Wiener index in the Table 7 uses a polynomial based on the benzenoid classification, namely linear, zig-zag, helix, and others. If we recall the definition of the Wiener index, namely the sum of the distances between any two carbon atoms in the molecule in terms of carbon-carbon bonds (Bonchev *et al.*, [43]). We call the path number of the graph G, the Wiener index of G is:

$$W(G) = \sum_{i,j} \frac{D_{ij}(G)}{2}. \tag{35}$$

Its element $D_{ij}(G)$ represent the length of the shortest path (the topological distance) between ith and jth vertices of G. All elements of type $D_{ij}(G)$ are, by definition, zero. Also by definition, $D_{ij}(G) = 1$ for i, j-neighbors. Thus, all the entries of the topological distance matrix are integers. In another words, $W(G)$ represents the sum of all the topological distance in the graph. As an illustration the distance matrix of the L_1 graph is shown below:



$$D(G) = \begin{bmatrix} 0 & 1 & 2 & 3 & 3 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 3 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix}; \; W(G) = 28.$$

Due to symmetry of the distance matrix each distance D_{ij} between ith and jth vertices of G is counted twice in it. Hence, in order to avoid redundancy, it is sufficient to consider the triangular off-diagonal submatrix only. So using the distance matrix, we get that the Wiener index for one hexagonal cycle is 28. Now let's use the cubic polynomials of Bonchev *et al.*, [43], and Dobrynin *et al.*, [42]. We get the cubic polynomial as follows:

$$W(L_1) = \frac{(16\left(1\right)^3 + 36\left(1\right)^2 + 26\left(1\right) + 3\right)}{3} = 27.$$

From the calculation of the cubic polynomial, we can see that the results are very close to those of manual calculations. Therefore, this method is very suitable and good for the calculation of the corresponding benzenoid compounds. This also applies to the calculation of other benzenoid compounds in Table 7.

4. Conclusion

In this paper, various methods of calculating the value of the Wiener index have been discussed. Then, we also calculated the Wiener index values of several benzenoid compounds using cubic polynomial. This method is very suitable because the results of cubic polynomial

calculations are very close to the results of manual calculations, as has been demonstrated. The calculated benzenoid compounds are compounds that are very useful in drug design in the pharmaceutical field. Research on more complex benzenoid compounds still needs to be developed because there is no specific research on the relationship between the Wiener index and the eigenvalues. This research has a great opportunity to show the relationship between each Wiener index formula and its eigenvalues.

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