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Wiener Index of Annihilator Graphs and their Properties

R.P. Somani

Department of Mathematics, Government College, Kota, Rajasthan, India

ABSTRACT: Topological indices have received special attention in mathematical chemistry. These are invariants which can be calculated from the underlying molecular graphs and exhibit good correlations with physical and chemical properties of the corresponding molecules. Molecules and molecular compounds are often modeled by the molecular graph. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Topological indices are used for correlation analysis in theoretical chemisty, pharmacology, toxicology, and environmental chemistry. There are two major classes of topological indices namely distance-based topological indices and degree-based topological indices of graphs. Among these, the classes of distance-based topological indices play a vital role in chemical graph theory. One of the well studied distance-based topological index is called Wiener index of graph.

KEYWORDS-wiener, index, graph, annihilator, properties, topological

I. INTRODUCTION

Wiener index of graphs

The Wiener index was introduced by Harold Wiener [Citation38] in 1947. Wiener index has remarkable variety of chemical applications. Wiener himself used it to predict boiling point of parafin. He named this index as path number. Later on, the path number was renamed as the Wiener index.[1,2,3] The Wiener index is considered as one of the most used topological indices which highly correlates many physical and chemical properties of molecular compounds. In particular, the Wiener index has a variety of applications in pharmaceutical science and in the structure of nanotubes. For results and applications of Wiener index, Based on this interest on Wiener index some other topological indices have also been discovered. The mathematical representation of Wiener index was given by Hosoya .[7,8,9]

In the past three decades, graphs constructed from algebraic structures have been studied extensively by many authors and have become a major field of research. The idea of constructing a graph from an algebraic structure was introduced by Arthur Cayley in 1878. He constructed a graph from groups. Another important graph construction is the construction of graphs from rings. The study of graphs from rings contributes to the interplay between the ring structure and the derived graph structure. One can sometimes translate algebraic properties of commutative rings to graph-theoretic language, and then the geometric properties of the graphs can help explore some interesting results related to commutative rings. The study of graphs from rings starts from the most well-studied zero-divisor graphs from commutative rings. The other well-studied graphs on the subject concentrated in this article are total graphs, unit graphs and prime graphs.[5,7] For more details on graphs from rings, one may refer . The Wiener index may be calculated directly using an algorithm for computing all pairwise distances in the graph. When the graph is unweighted (so the length of a path is just its number of edges), these distances may be calculated by repeating a breadth-first search algorithm, once for each starting vertex.[13] The total time for this approach is O(nm), where n is the number of vertices in the graph and m is its number of edges.

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For weighted graphs, one may instead use the Floyd–Warshall algorithm[13][14][15] or Johnson's algorithm,[16] with running time $O(n^3)$ or $O(nm + n^2 \log n)$ respectively. Alternative but less efficient algorithms based on repeated matrix multiplication have also been developed within the chemical informatics literature.[17][18]

When the underlying graph is a tree (as is true for instance for the alkanes originally studied by Wiener), the Wiener index may be calculated more efficiently. If the graph is partitioned into two subtrees by removing a single edge e, then its Wiener index is the sum of the Wiener indices of the two subtrees, together with a third term representing the paths that pass through e. This third term may be calculated in linear time by computing the sum of distances of all vertices from e within each subtree and multiplying the two sums.[19] This divide and conquer algorithm can be generalized from trees to graphs of bounded treewidth, and leads to near-linear-time algorithms for such graphs.[20]

An alternative method for calculating the Wiener index of a tree, by Bojan Mohar and Tomaž Pisanski, works by generalizing the problem to graphs with weighted vertices, where the weight of a path is the product of its length with the weights of its two endpoints.[10,11,12] If v is a leaf vertex of the tree then the Wiener index of the tree may be calculated by merging v with its parent (adding their weights together), computing the index of the resulting smaller tree, and adding a simple correction term for the paths that pass through the edge from v to its parent. By repeatedly removing leaves in this way, the Wiener index may be calculated in linear time.[13]

For graphs that are constructed as products of simpler graphs, the Wiener index of the product graph can often be computed by a simple formula that combines the indices of its factors.[21] Benzenoids (graphs formed by gluing regular hexagons edge-to-edge) can be embedded isometrically into the Cartesian product of three trees, allowing their Wiener indices to be computed in linear time by using the product formula together with the linear time tree algorithm.[22]

Inverse problem

Gutman & Yeh (1995) considered the problem of determining which numbers can be represented as the Wiener index of a graph.[23] They showed that all but two positive integers have such a representation; the two exceptions are the numbers 2 and 5, which are not the Wiener index of any graph. For graphs that must be bipartite, they found that again almost all integers can be represented, with a larger set of exceptions: none of the numbers in the set[13,15,17]

{2, 3, 5, 6, 7, 11, 12, 13, 15, 17, 19, 33, 37, 39}

can be represented as the Wiener index of a bipartite graph.

Gutman and Yeh conjectured, but were unable to prove, a similar description of the numbers that can be represented as Wiener indices of trees, with a set of 49 exceptional values:

2, 3, 5, 6, 7, 8, 11, 12, 13, 14, 15, 17, 19, 21, 22, 23, 24, 26, 27, 30, 33, 34, 37, 38, 39, 41, 43, 45, 47, 51, 53, 55, 60, 61, 69, 73, 77, 78, 83, 85, 87, 89, 91, 99, 101, 106, 113, 147, 159 (sequence A122686 in the OEIS)

The conjecture was later proven by Wagner, Wang, and Yu.[24][25]

In mathematics, the Wiener series, or Wiener G-functional expansion, originates from the 1958 book of Norbert Wiener. It is an orthogonal expansion for nonlinear functionals closely related to the Volterra series and having the same relation to it as an orthogonal Hermite polynomial expansion has to a power series. For this reason it is also known as the Wiener–Hermite expansion. The analogue of the coefficients are referred to as Wiener kernels. The terms of the series are orthogonal (uncorrelated) with respect to a statistical input of white noise. This property allows the terms to be identified in applications by the Lee–Schetzen method.[18,19,20]

The Wiener series is important in nonlinear system identification. In this context, the series approximates the functional relation of the output to the entire history of system input at any time. The Wiener series has been applied mostly to the identification of biological systems, especially in neuroscience.

The name Wiener series is almost exclusively used in system theory. In the mathematical literature it occurs as the Itô expansion (1951) which has a different form but is entirely equivalent to it.

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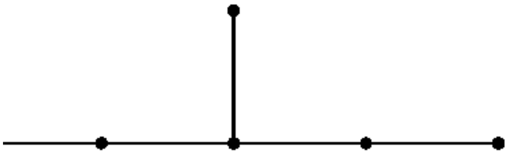
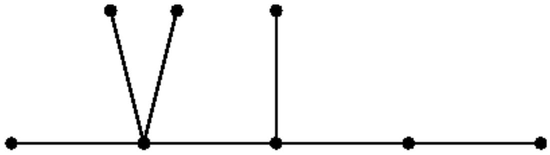
The Wiener series should not be confused with the Wiener filter, which is another algorithm developed by Norbert Wiener used in signal processing.[21,22,23]

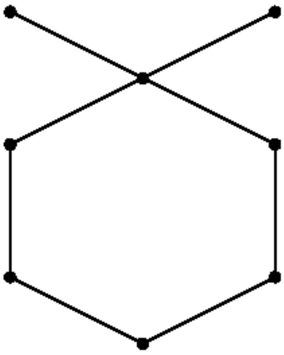
II. DISCUSSION



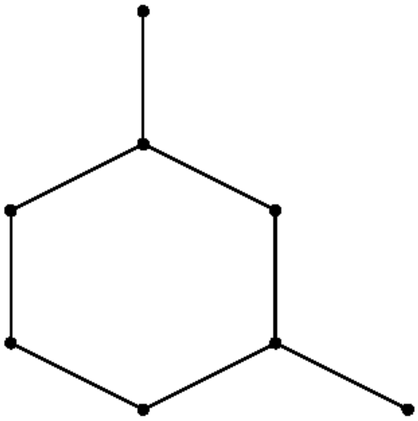
a) Tree with Wiener index 31.



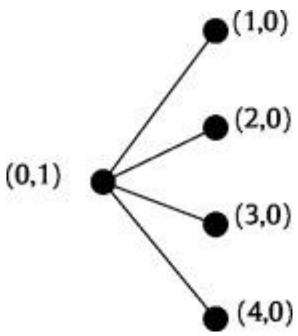
(b) Tree with Wiener index 63.



(c) Bipartite graph with Wiener index 59.



(d) Bipartite graph with Wiener index 61.



The Wiener index of the zero-divisor graph of a finite commutative ring with unity

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The following table summarizes values of the Wiener index for various special classes of graphs.[20,21]

graph class	OEIS	, , ...
Andrásfai graph	A292018	1, 15, 44, 88, 147, 221, 310, 414, ...
antelope graph	A292039	0, , , , , , , 11548, 16660, ...
antiprism graph	A002411	X, X, 18, 40, 75, 126, 196, 288, ...
Apollonian network	A289022	6, 27, 204, 1941, 19572, 198567, ...
black bishop graph	A292051	0, 1, 14, 42, 124, 251, 506, 852, 1432, 2165, ...
cocktail party graph	A001105	, 8, 18, 32, 50, 72, 98, 128, 162, ...
complete bipartite graph	A000567	1, 1, 5, 73, 2069, 95401, 6487445, ...
complete tripartite graph	A094159	1, 11, 1243, 490043, 463370491, ...
complete graph	A000217	0, 1, 3, 6, 10, 15, 21, 28, 36, ...
-crossed prism graph	A292018	X, 48, 132, 288, 540, 912, 1428, ...
crown graph	A033428	X, X, 27, 48, 75, 108, 147, 192, 243, ...
cube-connected cycle graph	A292028	X, X, 888, 9472, 76336, 559584, 3594952, ...
cycle graph	A034828	X, X, 3, 8, 15, 27, 42, 64, 90, ...
Fibonacci cube graph	A238419	1, 4, 16, 54, 176, 548, 1667, 4968,, ...
fiveleaper graph	A292040	0, , , , , , , 6364, 9888, 15216, ...
folded cube graph	A292029	X, 1, 6, 40, 200, 1056, 4928, 23808, ...
gear graph	A049598	X, X, 36, 72, 120, 180, 252, 336, 432, ...
grid graph	A143945	0, 8, 72, 320, 1000, 2520, 5488, 10752, ...
grid graph	A292045	0, 48, 972, 7680, 37500, 136080, 403368, ...
halved cube graph	A292044	0, 1, 6, 32, 160, 768, 3584, 16384, ...
Hanoi graph	A290004	3, 72, 1419, 26580, 487839, 8867088, ...

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hypercube graph	A002697	1, 8, 48, 256, 1280, 6144, 28672, ...
Keller graph	A292056	, 200, 2944, 43392, 650240, 9889792, ...
king graph	A292053	0, 6, 52, 228, 708, 1778, 3864, 7560, ...
knight graph	A292054	0, , , 288, 708, 1580, 3144, 5804, 9996, ...
Menger sponge graph	A292036	612, 794976, 954380016, ...
Möbius ladder	A180857	X, X, 21, 44, 85, 138, 217, 312, 441, ...
Mycielski graph	A292055	0, 1, 15, 90, 435, 1926, 8175, 33930, ...
odd graph	A136328	0, 3, 75, 1435, 25515, 436821, ...
pan graph	A180861	8, 16, 26, 42, 61, 88, 119, 160, 206, 264, ...
path graph	A000292	0, 1, 4, 10, 20, 35, 56, 84, 120, ...
permutation star graph	A284039	0, 1, 27, 744, 26520, 1239840, ...
prism graph	A138179	X, X, 21, 48, 85, 144, 217, 320, 441, ...
queen graph	A292057	0, 6, 44, 164, 440, 970, 1876, 3304, 5424, ...
rook graph	A085537	X, 8, 54, 192, 500, 1080, 2058, 3584, 5832, ...
rook complement graph	A292058	0, , 54, 168, 400, 810, 1470, 2464, ...
Sierpiński carpet graph	A292025	64, 13224, 2535136, 485339728, ...
Sierpiński gasket graph	A290129	3, 21, 246, 3765, 64032, 1130463, 20185254, ...
Sierpiński tetrahedron graph	A292026	6, 66, 1476, 42984, 1343568, 42744480, ...
star graph	A000290	0, 1, 4, 9, 16, 25, 36, 49, 64, ...
sun graph	A180863	X, X, 21, 44, 75, 114, 161, 216, 279, 350, ...
sunlet graph	A180574	X, X, 27, 60, 105, 174, 259, 376, 513, 690, ...
tetrahedral graph	A292061	X, X, X, X, X, 300, 1050, 2940, 7056, 15120, ...
torus grid graph	A122657	54, 256, 750, 1944, 4116, 8192, 14580, 25000, ...

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transposition graph	A292062	0, 1, 21, 552, 19560, 920160, 55974240, ...
triangular graph	A006011	0, 3, 18, 60, 150, 315, 588, 1008, 1620, ...
triangular grid graph	A112851	3, 21, 81, 231, 546, 1134, 2142, 3762, 6237, ...
web graph	A180576	X, X, 69, 148, 255, 417, 616, 888, 1206, 1615, ...
wheel graph	A002378	X, X, X, X, 12, 20, 30, 42, 56, 72, ...
white bishop graph	A292059	X, 1, 8, 42, 104, 251, 464, 852, 1360, 2165, ...

III. RESULTS

But there is some ambiguity in the mathematical modelling of unsaturated hydrocarbons. In one of the seminal papers on the prediction of physico-chemical properties from topological indices by Basak et al. [5] three different clusters of hydrocarbons were investigated: alkanes, alkylbenzenes and polycyclic aromatic hydrocarbons, all of them modelled with a simple graph although the last two groups of molecules contain double CC bonds. We are interested in the correlation between the weighted Wiener index and the boiling points of alkenes and alkadienes. The aim of this paper is to mathematically model an unsaturated hydrocarbon with an edge-weighted graph, then calculate the corresponding distances in the graph and obtain a new Wiener index. With the use of the QSPR (Quantitative Structure Property Relationships) we show that the new Wiener index gives very good predictions of the boiling points of alkenes and alkadienes.[19,20] This approach can be applied in the calculation of different distance-based topological indices for unsaturated hydrocarbons as well as for organic compounds in general. At the end, we compare our method for a group of considered molecules with the method used in References . The Wiener index W(G) of a connected graph G is a sum of distances between all pairs of vertices of G. In 1991, Šoltés formulated the problem of finding all graphs G such that for every vertex v the equation W(G)=W(G−v) holds. The cycle C11 is the only known graph with this property. In this paper we consider the following relaxation of the original problem: find a graph with a large proportion of vertices such that removing any one of them does not change the Wiener index of a graph. As the main result, we build an infinite series of graphs with the proportion of such vertices tending to 1/2.

Topological indices are graph invariants computed usually by means of the distances or degrees of vertices of a graph. In chemical graph theory, a molecule can be modeled by a graph by replacing atoms by the vertices and bonds by the edges of this graph. Topological graph indices have been successfully used in determining the structural properties and in predicting certain physicochemical properties of chemical compounds. Wiener index is the oldest topological index which can be used for analyzing intrinsic properties of a molecular structure in chemistry. The Wiener index of a graph G is equal to the sum of distances between all pairs of vertices of G. Recently, the entire versions of several indices have been introduced and studied due to their applications. Here we introduce the entire Wiener index of a graph. Exact values of this index for trees and some graph families are obtained, some properties and bounds for the entire Wiener index are established. Exact values of this new index for subdivision and λ-subdivision graphs and some graph operations are obtained.[17,18,19]

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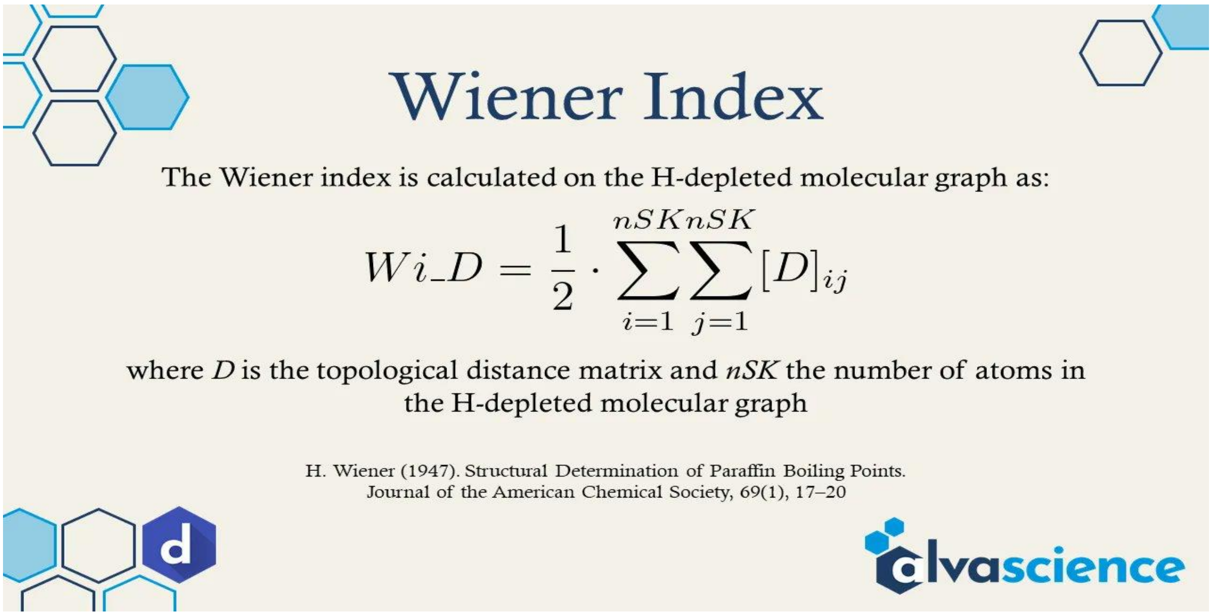

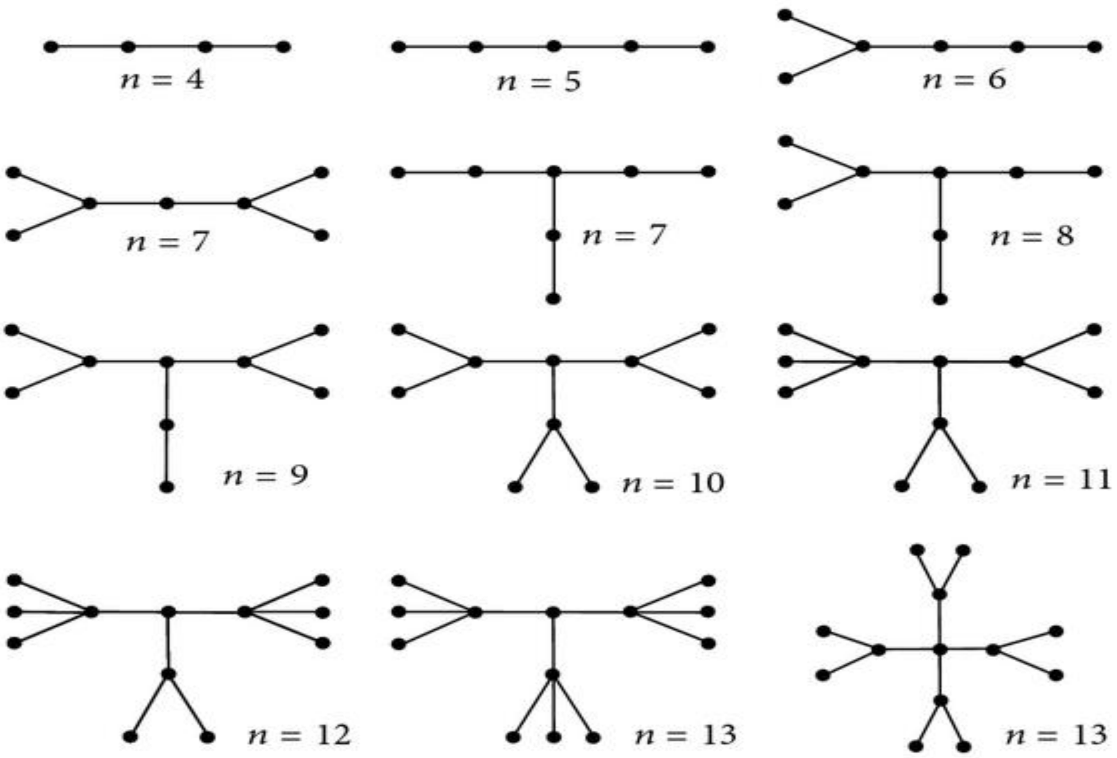

Weiner index of graph with radius 2

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IV. CONCLUSION

The Wiener index W(G) of a graph G is a distance-based topological index defined as the sum of distances between all pairs of vertices in G. It is shown that for λ=2 there is an infinite family of planar bipartite chemical graphs G of girth 4 with the cyclomatic number λ, but their line graphs are not chemical graphs, and for λ⩾2 there are two infinite families of planar nonbipartite graphs G of girth 3 with the cyclomatic number λ; the three classes of graphs have the property W(G)=W(L(G)), where L(G) is the line graph of G.[20,21,22,23]

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