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COMPARATIVE ANALYSIS BETWEEN SZEGED INDEX AND THE WIENER INDEX

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Abstract

Topological indices are numerical quantities in graph theory that can be obtained from any type of graphical structure. The molecular structures of hexane, heptane, and the octane isomers are being converted into numbers with the use of topological indices. The physical characteristics of the structural isomers of the alkanes, hexane, heptane, and octane, are used to compute the distance-based topological indices of Wiener, Szeged, and mostar. The link between the three topological indices and the physical characteristics of the structural isomers of the alkanes is calculated in this article. The correlation value between the distance-based topological indices and the physical parameters of melting point (Mp), surface tension (St), heats of vaporisation (Hv), boiling point (Bp), and molar volume (Mv) is here determined using the correlation approach.In this work, we calculate the relationship between the physical characteristics of the structural isomers of the alkanes and the distance-based topological indices. Additionally, we determine which indices are most useful in predicting the physical characteristics of the structural isomers of alkanes.

Key words: Szeged Index, Wiener Index, Mostar Index, Distance, Correlation

Introduction

Vertices and edges are thought of as the components of a graph.Atoms are represented as vertices and bonds as edges in molecular graphs. Molecular graphs are treated as integers in topological indices.Basically, the molecular structures are converted into numbers using topological indices based on degree and distance. A distance in a graph G is the length of the shortest path that connects the vertices u and v. A degree of G is defined as the quantity of edges that intersect the vertex. The three different distance-based topological indices of the Szeged, Wiener, and Mostar indexes are used in this study. A graph G's szeged index can be calculated

by multiplying the number of vertices that are closer to u than v by the total number of vertices that are closer to v than u. The total of the differences between the number of vertices that are closer to u than v and the number that are closer to v than u is the wiener index for a given graph. The first thing we're doing is computing the values of the hexane, heptane, and octane isomers of the following alkanes for the three topological indices. Next, we are calculating the correlation between the physical characteristics of the structural isomers of the alkanes and the three topological indices. This research identifies the topological indices that have a strong correlation with the physical characteristics of alkanes. In light of this, we may finally draw the conclusion that one of the indices accurately predicts the physical characteristics of the structural isomers of alkanes.

Definition: A graph's Wiener index

The total distance between each pair of vertices in a graph G is said to be the wiener index of that graph (Gi). It's represented by W(G).

$$W(G) = \sum_{(u,v)\subseteq V(G)} d(u,v) .$$

The notation d(u,v) represents the distance between each vertex in G.

Definition: Szeged index of a graph

An index of szeged graphs, the number of vertices that are closer to u than v and the number of vertices that are closer to v than u are added together to form G. It is denoted by

$$Sz(G).Sz(G) - \sum_{(u,v)\in E(G)} nunv$$

Definition: Mostar index of a graph

The sum of the differences between the number of vertices closer to u than v and the number of vertices closer to v than u is known as the mostar index of a graph G.It's indicated by

$$Sz(G).M\ o(G) = \sum_{(u,v)\in E(G)} |nu - nv|$$

Materials and methods

Alkanes' physical characteristics include their boiling point (Bp), molar volume (Mv), molar refraction (Mr), heats of vaporisation (Hv), surface tension (St), and melting point (Mp) are listed in table 1,2,3. The main formulas for the topological indices are as follows

1. $W(G) = \sum_{(u,v)\subseteq V(G)} d(u,v)$
2. $Sz(G) = \sum_{(u,v)\in E(G)} nunv$
3. $M\ o(G) = \sum_{(u,v)\in E(G)} |nu - nv|$

Table: 1

It shows that the physical properties of alkanes hexane, heptane and octane isomer

Alkanes	Bp	Mv	Mr	Hv	St	Mp
Hexane	68.740	130.688	29.9066	31.55	18.4	-95.35
2-methyl pentane	60.271	131.933	29.9459	29.86	17.3	-153.67
3-methyl pentane	63.282	129.717	29.8016	30.27	18.1	-118
2,2 methyl butane	49.741	132.744	29.9347	27.69	16.3	-99.87
2,3 dimethyl butane	57.988	130.240	29.8104	29.12	17.3	-128.54

Alkanes	Bp	Mv	Mr	Hv	St	Mp
Heptane	98.427	146.540	34.5504	36.55	20.2	-90.61
2-methyl hexane	90.052	147.656	34.5908	34.80	19.2	-118.28
3-methyl hexane	91.850	145.821	34.4597	35.08	19.7	-119.40
3-ethyl pentane	93.475	143.517	34.2827	35.22	20.4	-118.60
2,2-dimethylpentane	79.197	148.695	34.6166	32.43	18.0	-123.81
2,3-dimethyl pentane	89.784	144.153	34.3237	34.24	19.9	-119.10
2,4-dimethyl pentane	80.500	148.949	34.6192	32.88	18.1	-119.24
3,3-dimethyl pentane	86.064	144.530	34.3323	33.02	19.5	-134.46
2,2,3 trimethyl butane	81	-	-	-	-	-

Alkanes	Bp	Mv	Mr	Hv	St	Mp
octane	125.665	-56.79	162.592	41.48	21.7	-56.79
2-methyl heptane	117.647	-109.04	163.663	39.68	20.6	-109.04
3-methyl heptane	118.925	-120.50	161.832	39.83	21.1	-120.50
4-methyl heptane	117.709	-120.95	162.105	39.67	21.0	-120.95
3-ethylhexane	118.53	-	160.07	39.40	21.5	-
2,2-dimethylhexane	110.84	-121.18	164.28	37.29	19.6	-121.18
2,3-dimethylhexane	115.607		160.39	38.79	20.9	-
2,4dimethylhexane	109.10	-137.50	163.09	37.76	20.0	-137.50
2,5-dimethylhexane	111.96	-91.20	164.69	37.86	19.7	-91.20
3,3-dimethylhexane	117.72	-126.10	160.87	37.93	20.6	-126.10
3,4--dimethylhexane	115.65	-	158.81	39.02	21.6	-
3-ethyl2-mrthylpentane	118.25	-114.96	158.79	38.52	21.5	-114.96
3-ethyl3-mrthylpentane	109.84	-90.87	157.02	37.99	21.9	-90.87
2,2,3trimethylpentane	99.23	-112.27	159.52	36.91	20.6	-112.27
2,2,4trimethylpentane	114.76	-107.38	165.08	35.13	18.7	-107.38
2,3,3 trimethylpentane	113.5	-100.7	157.29	37.22	21.5	-100.7
2,3,4trimethylpentane	113.46	-	-	37.75	-	-
2,2,3,3 trimethylpentane	106.5	-109.21	158.85	37.61	21.1	-109.21

Table: 2

It shows that the calculated values for the topological indices of mostar index, wiener index and szeged index

Alkanes	Wiener index	Mostar index	Szeged index
Hexane	35	12	10
2-methyl pentane	31	16	7
3-methyl pentane	32	14	6
2,2 methyl butane	29	16	3
2,3 dimethyl butane	28	18	4

Alkanes	Wiener index	Mostar index	Szeged index
Heptane	56	18	20
2-methyl hexane	52	20	16
3-methyl hexane	50	22	14
3-ethyl pentane	46	24	12
2,2-dimethylpentane	46	24	10
2,3-dimethyl pentane	48	22	10
2,4-dimethyl pentane	44	26	12
3,3-dimethyl pentane	48	24	8
2,2,3trimethyl butane	42	26	6

Alkanes	Wiener index	Mostar index	Szeged index
Octane	84	24	35
2-methyl heptanes	79	26	30
3-methyl heptanes	76	30	27
4-methyl heptanes	75	30	26
3-ethylhexane	72	32	23
2,2-dimethylhexane	71	30	22
2,3-dimethylhexane	70	32	30
2,4dimethylhexane	71	30	22
2,5-dimethylhexane	74	28	25
3,3-dimethylhexane	67	34	18
3,4—dimethylhexane	68	32	19
3-ethyl2-mrthylpentane	67	34	18
3-ethyl3-mrthylpentane	64	36	15
2,2,3trimethylpentane	63	34	14
2,2,4trimethylpentane	66	32	17
2,3,3 trimethylpentane	62	36	13
2,3,4trimethylpentane	65	34	16
2,2,3,3 trimethylpentane	58	30	09

Table: 3

The physical properties and the calculated values for alkanes are listed in this table

Alkanes	Wiener index	Mostar index	Szeged index	Bp	Mv	Mr	Hv	St	Mp
Hexane	35	12	10	68.740	130.688	29.9066	31.55	18.4	-95.35
2-methyl pentane	31	16	7	60.271	131.933	29.9459	29.86	17.3	-153.67
3-methyl pentane	32	14	6	63.282	129.717	29.8016	30.27	18.1	-118
2,2 methyl butane	29	16	3	49.741	132.744	29.9347	27.69	16.3	-99.87
2,3 dimethyl butane	28	18	4	57.988	130.240	29.8104	29.12	17.3	-128.54

Alkanes	Wiener index	Mostar index	Szeged index	Bp	Mv	Mr	Hv	St	Mp
Heptane	56	18	20	98.427	146.540	34.5504	36.55	20.2	-90.61
2-methyl hexane	52	20	16	90.052	147.656	34.5908	34.80	19.2	-118.28
3-methyl hexane	50	22	14	91.850	145.821	34.4597	35.08	19.7	-119.40
3-ethyl pentane	46	24	12	93.475	143.517	34.2827	35.22	20.4	-118.60
2,2-dimethylpentane	46	24	10	79.197	148.695	34.6166	32.43	18.0	-123.81
2,3-dimethyl pentane	48	22	10	89.784	144.153	34.3237	34.24	19.9	-119.10
2,4-dimethyl pentane	44	26	12	80.500	148.949	34.6192	32.88	18.1	-119.24
3,3-dimethyl pentane	48	24	8	86.064	144.530	34.3323	33.02	19.5	-134.46
2,2,3 trimethyl butane	42	26	6	81	-	-	-	-	-

Alkanes	Wiener index	Mostar index	Szeged index	Bp	Mv	Mr	Hv	St	Mp
Octane	84	24	35	125.665	-56.79	162.592	41.48	21.7	-56.79
2-methyl heptane	79	26	30	117.647	-109.04	163.663	39.68	20.6	-109.04
3-methyl heptane	76	30	27	118.925	-120.50	161.832	39.83	21.1	-120.50
4-methyl heptane	75	30	26	117.709	-120.95	162.105	39.67	21.0	-120.95
3-ethylhexane	72	32	23	118.53	-	160.07	39.40	21.5	-
2,2-dimethylhexane	71	30	22	110.84	-121.18	164.28	37.29	19.6	-121.18
2,3-dimethylhexane	70	32	30	115.607		160.39	38.79	20.9	-
2,4dimethylhexane	71	30	22	109.10	-137.50	163.09	37.76	20.0	-137.50
2,5-dimethylhexane	74	28	25	111.96	-91.20	164.69	37.86	19.7	-91.20
3,3-dimethylhexane	67	34	18	117.72	-126.10	160.87	37.93	20.6	-126.10
3,4--dimethylhexane	68	32	19	115.65	-	158.81	39.02	21.6	-
3-ethyl2-mrthylpentane	67	34	18	118.25	-114.96	158.79	38.52	21.5	-114.96
3-ethyl3-mrthylpentane	64	36	15	109.84	-90.87	157.02	37.99	21.9	-90.87
2,2,3trimethylpentane	63	34	14	99.23	-112.27	159.52	36.91	20.6	-112.27
2,2,4trimethylpentane	66	32	17	114.76	-107.38	165.08	35.13	18.7	-107.38
2,3,3 trimethylpentane	62	36	13	113.5	-100.7	157.29	37.22	21.5	-100.7
2,3,4trimethylpentane	65	34	16	113.46	-	-	37.75	-	-
2,2,3,3 trimethylpentane	58	30	09	106.5	-109.21	158.85	37.61	21.1	-109.21

Table: 4

It demonstrates that the alkanes and topological indices' coefficient of association

Hexane	Bp	Mv	Mr	Hv	St	Mp
Sz(G)	0.9121	-0.295	0.4443	0.9433	0.8241	0.0838
W(G)	0.8439	-0.2739	0.4212	0.8781	0.8018	0.3331
M(G)	-0.7121	0.2245	-0.1421	-0.7456	-0.7061	-0.54

Heptane	Bp	Mv	Mr	Hv	St	Mp
Sz(G)	0.6703	0.2387	0.4315	0.8082	0.3198	0.8891
W(G)	0.7555	-0.1277	0.0416	0.7713	0.5096	0.7023
M(G)	-0.8032	0.077	-0.1302	-0.7924	-0.5261	-0.7244

Octane	Bp	Mv	Mr	Hv	St	Mp
Sz(G)	0.4569	0.2957	0.5429	0.6169	0.7678	0.0677
W(G)	0.4646	0.2957	0.5976	0.6709	0.74	-0.0055
M(G)	-0.3914	-0.3087	-0.6998	-0.5531	0.2219	-.03087

Table 4 shows a strong correlation between the Szeged index and the physical characteristics of alkanes when comparing the Wiener index. The physical parameters of boiling point, temperatures of vaporisation, and surface tension are significantly associated with the topological indices of Szeged and Wiener in the hexane isomer. The physical characteristics of melting point and temps of vaporisation are significantly associated with the topological indices of Szeged index in the hepane isomer. However, the topological indices of the Wiener index in the hepane isomer are only mild, and the alkanes' physical attributes have a negative correlated value. The physical characteristics of the heptanes isomer do not exhibit a strong association with the Wiener index. The correlation between the physical parameters of the octane isomer and the topological indices of Szeged and Wiener index is only moderate. For every alkane, there isn't a single highly linked value in the mostar index. According to the majority of results when comparing the Szeged and Wiener indices, the Szeged index performs the best when determining the physical characteristics of all alkanes.

Conclusion:

In this study, we computed the Szeged, Wiener, and Mostar distance-based topological indices. We also examined the correlation between the topological indices' values and the physical characteristics of alkanes, specifically the hexane, heptane, and octane isomers. It is evident that the Szeged index, when compared to the Wiener index, accurately predicts the physical and chemical properties of alkanes. Thus, in the end, we determine that the Szeged index is the best index for estimating the chemical and physical characteristics of alkanes.

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