**JOURNAL OF ALGEBRAIC STATISTICS**
Volume 13, No. 2, 2022, p. 3338-3345
https://publishoa.com
ISSN: 1309-3452

# The Physical-Chemical Characteristics of Alkanes and Wiener Indices

**M. Puruchothama Nayaki[a] and F. Simon raj[b]**

[a]Department of Mathematics, Dhanraj Baid Jain College, Chennai -600 097, Tamilnadu, India.
[b]Department of Mathematics, Hindustan Institute of Technology and Science, Chennai, 603103, Tamilnadu, India.

**Received** 2022 March 25; **Revised** 2022 April 28; **Accepted** 2022 May 15.

**Abstract**

The QSPR analysis of the distance-based topological indices Wiener, Terminal, and Hyper Wiener is discovered for 67 alkanes,. The eight physicochemical qualities of 67 alkanes and the three different types of Wiener index values are connected to predict the physicochemical features of structural isomers of alkanes. In this study, the QSPR method is used to analyse alkane characteristics for indices.

**Keywords**: QSPR, Alkanes, Wiener index, Terminal Wiener index and Hyper Wiener index, correlation coefficient

## Introduction

The Queen of Mathematics is graph theory. There are vertices and edges in a linear graph. A molecular graph in chemical graph theory is a graph-theoretical representation of the structural formula of a chemical molecule. Numerous topological indices are dealt with in graph theory. The highly anticipated physicochemical features of all sorts of alkanes are found using the distance-based topological indices known as the Wiener index, Terminal Wiener index, and Hyper Wiener index. The level of prediction for the physicochemical characteristics of alkanes is evaluated by computing the coefficient of correlation between the three types of Wiener indices and the physicochemical properties of 67 alkanes.

## Basic definition

The first index used to determine distance-based topological indices is the Wiener index. Harry Wiener, who first invented the Wiener index in 1947, received its name. The Wiener index, which measures molecular distance, is also the oldest topological index. Suppose G is a connected graph. The Wiener index of a connected graph G is denoted by W(G) and is defined by

$$W(G= \sum_{u,v\in V(G)} \quad dG(u, v)$$

Where dG(u,v) is the distance between the vertices u and v.

## Terminal Wiener index

A linked graph, G, shall exist. The total of the distances between all pairs of a graph G's pendent vertices is known as the graph's terminal Wiener index.

Terminal Wiener index

$$TW(G) =\sum_{1\le i<j\le k} \quad d(u, v \backslash G)$$

## Hyper Wiener index

Hyper Wiener index was introduced by Milan Randic in 1993.This index is applied for trees. The Hyper Wiener index is denoted by $HW(G) = 1/2\sum [ dG(u, v)+dG^2(u, v) ]$

**JOURNAL OF ALGEBRAIC STATISTICS**
Volume 13, No. 2, 2022, p. 3338-3345
https://publishoa.com
ISSN: 1309-3452

**The uses of Distance based topological indices in QSPR studies**

The eight physicochemical properties [boiling point (Bp), molar volume (Mv) at 20 c, molar fractions (Mr), at 20 c, heats of vaporisation (hv) at 25 c, surface tensions (St) at 20 c, and melting points (Mp) of 67 alkanes from n butanes to nonane are used in this paper along with the three types of distance-based topological The eight physicochemical parameters of 67 alkanes as well as their property values are listed in table [1] in Dejan Plasvic et alstudy .'s from [25].

**Table 1**

The table 1 shows the 67 alkanes and its eight physico chemical properties

| S.No. | Alkane | bp($^{\circ}C$) | mv($cm^3$) | mr($cm^3$) | hv(kJ) | ct($^{\circ}C$) | cp(atm) | st(dyne/cm) | mp($^{\circ}C$) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Butane | -0.500 | | | | 152.01 | 37.47 | | -138.35 |
| 2 | 2-methylpropane | -11.730 | | | | 134.98 | 36 | | -159.60 |
| 3 | Pentane | 36.074 | 115.205 | 25.2656 | 26.42 | 196.62 | 33.31 | 16.00 | -129.72 |
| 4 | 2-methylbutane | 27.852 | 116.426 | 25.2923 | 24.59 | 187.70 | 32.9 | 15.00 | -159.90 |
| 5 | 2,2dimethylpropane | 9.503 | 112.074 | 25.7243 | 21.78 | 160.60 | 31.57 | | -16.55 |
| 6 | Hexane | 68.740 | 130.688 | 29.9066 | 31.55 | 234.70 | 29.92 | 18.42 | -95.35 |
| 7 | 2-methylpentane | 60.271 | 131.933 | 29.9459 | 29.86 | 224.90 | 29.95 | 17.38 | -153.67 |
| 8 | 3-methyalpentane | 63.282 | 129.717 | 29.8016 | 30.27 | 231.20 | 30.83 | 18.12 | -118.00 |
| 9 | 2,2-methylbutane | 49.741 | 132.744 | 29.9347 | 27.69 | 216.20 | 30.67 | 16.30 | -99.87 |
| 10 | 2,3-dimethylbutane | 57.988 | 130.240 | 29.8104 | 29.12 | 227.10 | 30.99 | 17.37 | -128.54 |
| 11 | Heptanes | 98.427 | 146.540 | 34.5504 | 36.55 | 267.55 | 27.01 | 20.26 | -90.61 |
| 12 | 2-methylhexane | 90.052 | 147.656 | 34.5908 | 34.80 | 257.90 | 27.2 | 19.29 | -118.28 |
| 13 | 3-methylhexane | 91.850 | 145.821 | 34.4597 | 35.08 | 262.40 | 28.1 | 19.79 | -119.40 |
| 14 | 3-ethylpentane | 93.475 | 143.517 | 34.2827 | 35.22 | 267.60 | 28.6 | 20.44 | -118.60 |
| 15 | 2,2-dimethylpentane | 79.197 | 148.695 | 34.6166 | 32.43 | 247.70 | 28.4 | 18.02 | -123.81 |
| 16 | 2,3-dimethylpentane | 89.784 | 144.153 | 34.3237 | 34.24 | 264.60 | 29.2 | 19.96 | -119.10 |
| 17 | 2,4-dimethylpentane | 80.500 | 148.949 | 34.6192 | 32.88 | 247.10 | 27.4 | 18.15 | -119.24 |
| 18 | 3,3-dimethylpentane | 86.064 | 144.530 | 34.3323 | 33.02 | 263.00 | 30 | 19.59 | -134.46 |
| 19 | Octane | 125.665 | 162.592 | 39.1922 | 41.48 | 296.20 | 24.64 | 21.76 | -56.79 |
| 20 | 2-methylheptane | 117.647 | 163.663 | 39.2316 | 39.68 | 288.00 | 24.8 | 20.60 | -109.04 |
| 21 | 3-methylheptane | 118.925 | 161.832 | 39.1001 | 39.83 | 292.00 | 25.6 | 21.17 | -120.50 |
| 22 | 4-methylheptane | 117.709 | 162.105 | 39.1174 | 39.67 | 290.00 | 25.6 | 21.00 | -120.95 |
| 23 | 3-ethylhexane | 118.53 | 160.07 | 38.94 | 39.40 | 292.00 | 25.74 | 21.51 | |
| 24 | 2,2-dimethylhexane | 10.84 | 164.28 | 39.25 | 37.29 | 279.00 | 25.6 | 19.60 | -121.18 |
| 25 | 2,3-dimethylhexane | 115.607 | 160.39 | 38.98 | 38.79 | 293.00 | 26.6 | 20.99 | |

**JOURNAL OF ALGEBRAIC STATISTICS**
Volume 13, No. 2, 2022, p. 3338-3345
https://publishoa.com
ISSN: 1309-3452

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 26 | 2,4-dimethylhexane | 109.42 | 163.09 | 39.13 | 37.76 | 282.00 | 25.8 | 20.05 | -137.50 |
| 27 | 2,5-dimethylhexane | 109.10 | 164.69 | 39.25 | 37.86 | 279.00 | 25 | 19.73 | -91.20 |
| 28 | 3,3-dimethylhexane | 111.96 | 160.87 | 39.00 | 37.93 | 290.84 | 27.2 | 20.63 | -126.10 |
| 29 | 3,4-dimethylhexane | 117.72 | 158.81 | 38.84 | 39.02 | 298.00 | 27.4 | 21.64 | |
| 30 | 3-ethyl-2-methylpentane | 115.65 | 158.79 | 38.83 | 38.52 | 295.00 | 27.4 | 21.52 | -114.96 |
| 31 | 3-ethyl-3-methylpentane | 118.25 | 157.02 | 38.71 | 37.99 | 305.00 | 28.9 | 21.99 | -80.87 |
| 32 | 2,2,3-trimethylpentane | 109.84 | 159.52 | 38.92 | 36.91 | 294.00 | 28.2 | 20.67 | -112.27 |
| 33 | 2,2,4-trimethylpentane | 99.23 | 165.08 | 39.26 | 35.13 | 271.15 | 25.5 | 18.77 | -107.38 |
| 34 | 2,3,3-trimethylpentane | 114.76 | 157.29 | 38.76 | 37.22 | 303.00 | 29 | 21.56 | -100.70 |
| 35 | 2,3,4-trimethylpentane | 113.46 | 158.85 | 38.86 | 37.61 | 295.00 | 27.6 | 21.14 | -109.21 |
| 36 | Nonane | 150.79 | 178.71 | 43.84 | 46.44 | 322.00 | 22.74 | 22.92 | -53.52 |
| 37 | 2-methyloctane | 143.26 | 179.77 | 43.87 | 44.65 | 315.00 | 23.6 | 21.88 | -80.40 |
| 38 | 3-methyloctane | 144.18 | 177.95 | 43.72 | 44.75 | 318.00 | 23.7 | 22.34 | -107.64 |
| 39 | 4-methyloctane | 142.48 | 178.15 | 43.76 | 44.75 | 318.30 | 23.06 | 22.34 | -113.20 |
| 40 | 3-ethylheptane | 143.00 | 176.41 | 43.64 | 44.81 | 318.00 | 23.98 | 22.81 | -114.90 |
| 41 | 4-ethylheptane | 141.20 | 175.68 | 43.49 | 44.81 | 318.30 | 23.98 | 22.81 | |
| 42 | 2,2-dimethylheptane | 132.69 | 180.50 | 43.91 | 42.28 | 302.00 | 22.8 | 20.80 | -113.00 |
| 43 | 2,3-dimethylheptane | 140.50 | 176.65 | 43.63 | 43.79 | 315.00 | 23.79 | 22.34 | -116.00 |
| 44 | 2,4-dimethylheptane | 133.50 | 179.12 | 43.73 | 42.87 | 306.00 | 22.7 | 23.30 | |
| 45 | 2,5-dimethylheptane | 136.00 | 179.37 | 43.84 | 43.87 | 307.80 | 22.7 | 21.30 | |
| 46 | 2,6-dimethylheptane | 135.21 | 180.91 | 43.92 | 42.82 | 306.00 | 23.7 | 20.83 | -102.90 |
| 47 | 3,3-dimethylheptane | 137.300 | 176.897 | 43.6830 | 42.66 | 314.00 | 24.19 | 22.01 | |
| 48 | 3,4-dimethylheptane | 140.600 | 175.349 | 43.5473 | 43.84 | 322.70 | 24.77 | 22.80 | |
| 49 | 3,5-dimethylheptane | 136.000 | 177.386 | 43.6379 | 42.98 | 312.30 | 23.99 | 21.77 | |
| 50 | 4,4-dimethylheptane | 135.200 | 176.897 | 43.6022 | 42.66 | 317.80 | 24.18 | 22.01 | |

**JOURNAL OF ALGEBRAIC STATISTICS**
Volume 13, No. 2, 2022, p. 3338-3345
https://publishoa.com
ISSN: 1309-3452

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 51 | 3-ethyl-2-methylhexane | 138.000 | 175.445 | 43.6550 | 43.84 | 322.70 | 24.77 | 22.80 | |
| 52 | 4-ethyl-2-methylhexane | 133.800 | 177.386 | 43.6472 | 42.98 | 330.30 | 25.56 | 21.77 | |
| 53 | 3-ethyl-3-methylhexane | 140.600 | 173.077 | 43.2680 | 44.04 | 327.20 | 25.66 | 23.22 | |
| 54 | 2,2,4-trimethylhexane | 126.540 | 179.220 | 43.7638 | 40.57 | 301.00 | 23.39 | 20.51 | -120.00 |
| 55 | 2,2,5-trimethylhexane | 124.084 | 181.346 | 43.9356 | 40.17 | 296.60 | 22.41 | 20.04 | -105.78 |
| 56 | 2,3,3-trimethylhexane | 137.680 | 173.780 | 43.4347 | 42.23 | 326.10 | 25.56 | 22.41 | -116.80 |
| 57 | 2,3,4-trimethylhexane | 139.000 | 173.498 | 43.4917 | 42.93 | 324.20 | 25.46 | 22.80 | |
| 58 | 2,3,5-trimethylhexane | 131.340 | 177.656 | 43.6474 | 41.42 | 309.40 | 23.49 | 21.27 | -127.80 |
| 59 | 3,3,4-trimethylhexane | 140.460 | 172.055 | 43.3407 | 42.28 | 330.60 | 26.45 | 23.27 | -101.20 |
| 60 | 3,3-diethylpentane | 146.168 | 170.185 | 43.1134 | 43.36 | 342.80 | 26.94 | 23.75 | -33.11 |
| 61 | 2,2-dimethyl-3-ethylpentane | 133.830 | 174.537 | 43.4571 | 42.02 | 322.60 | 25.96 | 22.38 | -99.20 |
| 62 | 2,3-dimethyl-3-ethylpentane | 142.000 | 170.093 | 42.9542 | 42.55 | 338.60 | 26.94 | 23.87 | |
| 63 | 2,4-dimethyl-3-ethylpentane | 136.730 | 173.804 | 43.4037 | 42.93 | 324.20 | 25.46 | 22.80 | -122.20 |
| 64 | 2,2,3,3-tetramethylpentane | 140.274 | 169.495 | 43.2147 | 41.00 | 334.50 | 27.04 | 23.38 | -99.0 |
| 65 | 2,2,3,4-tetramethylpentane | 133.016 | 173.557 | 43.4359 | 41.00 | 319.60 | 25.66 | 21.98 | -121.09 |
| 66 | 2,2,4,4-tetramethylpentane | 122.284 | 178.256 | 43.8747 | 38.10 | 301.60 | 24.58 | 20.37 | -66.54 |
| 67 | 2,3,3,4-tetramethylpentane | 141.551 | 169.928 | 43.2016 | 41.75 | 334.50 | 26.85 | 23.31 | -102.12 |

**Table 2**

The table 2 shows the calculated value of 67 alkanes for the three types of Wiener indices

| **S.No.** | **Alkane** | ***W*(*G*)** | ***TW*(*G*)** | ***HW*(*G*)** |
|---|---|---|---|---|
| 1 | Butane | 10 | 3 | 46 |
| 2 | 2-methylpropane | 9 | 6 | 27 |
| 3 | Pentane | 20 | 8 | 146 |
| 4 | 2-methylbutane | 18 | 8 | 90 |
| 5 | 2,2dimethylpropane | 16 | 8 | 52 |
| 6 | Hexane | 35 | 5 | 371 |
| 7 | 2-methylpentane | 32 | 10 | 254 |
| 8 | 3-methyalpentane | 31 | 10 | 217 |
| 9 | 2,2-methylbutane | 26 | 15 | 142 |
| 10 | 2,3-dimethylbutane | 29 | 16 | 161 |
| 11 | Heptanes | 56 | 6 | 812 |

**JOURNAL OF ALGEBRAIC STATISTICS**
Volume 13, No. 2, 2022, p. 3338-3345
https://publishoa.com
ISSN: 1309-3452

| | | | | |
|---|---|---|---|---|
| 12 | 2-methylhexane | 52 | 12 | 604 |
| 13 | 3-methylhexane | 50 | 12 | 506 |
| 14 | 3-ethylpentane | 48 | 12 | 408 |
| 15 | 2,2-dimethylpentane | 49 | 16 | 370 |
| 16 | 2,3-dimethylpentane | 46 | 15 | 352 |
| 17 | 2,4-dimethylpentane | 48 | 16 | 426 |
| 18 | 3,3-dimethylpentane | 44 | 14 | 296 |
| 19 | Octane | 84 | 7 | 1596 |
| 20 | 2-methylheptane | 79 | 14 | 1261 |
| 21 | 3-methylheptane | 76 | 14 | 1072 |
| 22 | 4-methylheptane | 75 | 14 | 1011 |
| 23 | 3-ethylhexane | 72 | 14 | 822 |
| 24 | 2,2-dimethylhexane | 71 | 21 | 845 |
| 25 | 2,3-dimethylhexane | 71 | 22 | 766 |
| 26 | 2,4-dimethylhexane | 71 | 23 | 803 |
| 27 | 2,5-dimethylhexane | 74 | 24 | 962 |
| 28 | 3,3-dimethylhexane | 67 | 21 | 649 |
| 29 | 3,4-dimethylhexane | 68 | 22 | 668 |
| 30 | 3-ethyl-2-methylpentane | 67 | 22 | 607 |
| 31 | 3-ethyl-3-methylpentane | 64 | 21 | 514 |
| 32 | 2,2,3-trimethylpentane | 63 | 27 | 495 |
| 33 | 2,2,4-trimethylpentane | 66 | 32 | 606 |
| 34 | 2,3,3-trimethylpentane | 60 | 27 | 458 |
| 35 | 2,3,4-trimethylpentane | 65 | 32 | 551 |
| 36 | Nonane | 120 | 8 | 2892 |
| 37 | 2-methyloctane | 114 | 16 | 2388 |
| 38 | 3-methyloctane | 110 | 16 | 2076 |
| 39 | 4-methyloctane | 108 | 16 | 1920 |
| 40 | 3-ethylheptane | 105 | 16 | 1604 |

**JOURNAL OF ALGEBRAIC STATISTICS**
Volume 13, No. 2, 2022, p. 3338-3345
https://publishoa.com
ISSN: 1309-3452

| | | | | |
|---|---|---|---|---|
| 41 | 4-ethylheptane | 102 | 16 | 1452 |
| 42 | 2,2-dimethylheptane | 104 | 24 | 1718 |
| 43 | 2,3-dimethylheptane | 102 | 25 | 1548 |
| 44 | 2,4-dimethylheptane | 102 | 26 | 1524 |
| 45 | 2,5-dimethylheptane | 110 | 27 | 1646 |
| 46 | 2,6-dimethylheptane | 108 | 28 | 1926 |
| 47 | 3,3-dimethylheptane | 98 | 24 | 1340 |
| 48 | 3,4-dimethylheptane | 98 | 25 | 1298 |
| 49 | 3,5-dimethylheptane | 100 | 26 | 1396 |
| 50 | 4,4-dimethylheptane | 96 | 24 | 1218 |
| 51 | 3-ethyl-2-methylhexane | 96 | 25 | 1146 |
| 52 | 4-ethyl-2-methylhexane | 98 | 26 | 1244 |
| 53 | 3-ethyl-3-methylhexane | 92 | 24 | 992 |
| 54 | 2,2,4-trimethylhexane | 94 | 36 | 1108 |
| 55 | 2,2,5-trimethylhexane | 98 | 38 | 1328 |
| 56 | 2,3,3-trimethylhexane | 90 | 32 | 936 |
| 57 | 2,3,4-trimethylhexane | 92 | 36 | 992 |
| 58 | 2,3,5-trimethylhexane | 96 | 38 | 1188 |
| 59 | 3,3,4-trimethylhexane | 87 | 34 | 838 |
| 60 | 3,3-diethylpentane | 88 | 24 | 796 |
| 61 | 2,2-dimethyl-3-ethylpentane | 88 | 32 | 814 |
| 62 | 2,3-dimethyl-3-ethylpentane | 86 | 34 | 740 |
| 63 | 2,4-dimethyl-3-ethylpentane | 90 | 36 | 870 |
| 64 | 2,2,3,3-tetramethylpentane | 82 | 44 | 628 |
| 65 | 2,2,3,4-tetramethylpentane | 86 | 47 | 758 |
| 66 | 2,2,4,4-tetramethylpentane | 86 | 40 | 850 |
| 67 | 2,3,3,4-tetramethylpentane | 84 | 47 | 729 |

**JOURNAL OF ALGEBRAIC STATISTICS**
Volume 13, No. 2, 2022, p. 3338-3345
https://publishoa.com
ISSN: 1309-3452

**Table 3**

Table 3 displays the correlation coefficient between the eight physical-chemical characteristics of 67 alkanes and the three types of Wiener indices.

| TI | bp | mv | mr | hv | Ct | cp | st | mp |
|---|---|---|---|---|---|---|---|---|
| WI | 0.9378 | 0.8113 | 0.8533 | 0.8646 | 0.8946 | -0.9326 | 0.7221 | 0.4464 |
| TWI | -0.1582 | 0.5559 | 0.6082 | 0.5008 | 0.6505 | -0.4779 | 0.4846 | 0.1622 |
| HWI | -0.1782 | 0.6151 | 0.6338 | 0.6855 | 0.6385 | -0.8303 | 0.5080 | 0.3388 |

It is concluded that the Wiener index is highly predicted for the six physico-chemical properties of 67 alkanes. The TWI and HWI are not highly predicted for all the physico-chemical properties of 67 alkanes.

**Conclusion**

In this paper, A strong positive correlation value is explored from the calculated value of Wiener index and the eight physic-chemical properties. For the TW(G) and HW(G) moderate correlation value is found. It is concluded that Wiener index is suitable for predicting the physico chemical properties of 67 alkanes whereas TW(G) and HW(G) are not suitable for prediction.

**References:**

01. M.O. Albertson: The irregularity of a graph, Ars Comb**.,** 46(1997), 219–225
02. H. Abdo, S. Brandt, and D. Dimitrov: The total irregularity of a graph, Discrete Math. Theor. Comput. Sc,.16(2014), 201–206
03. T. Balban, Chemical applications of graph theory, Academic Press (1976).
04. K. Balakrishnan, B. Brešar, M. Chagat, S. Klavžar, A. Vesel, P. Žigertpleteršek Equal opportunity networks, distance-balanced graphs, and Wiener game, Discrete Optim. 12(2014), 150–154
05. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, Acta. Appl. Math. 66 (2001)211–249.
06. J. Devillers, A. T. Balban, Topological indices and related descriptors in QSAR and QSPR, Gordon and Breach SciencePublishers, Amsterdam, Netherlands, (1999).
07. A. Dobrynin, A. A. Kochetova, Degree-distance of a graph: A degree analogue of the Wiener index, J. Chem. Inf.Comput. Sci., 34 (1994) 1082–1086.
08. H. Dong, X. Guo, Ordering trees by their Wiener indices, MATCH Commun. Math. Comput. Chem. 56 (2006) 527–540.
09. T.Došli´C: Vertex-weighted Wiener polynomials for composite graphs, Ars Math. Contemp. 1(2008), 66–80.
10. Gutman, N. Trinajsti ´ c, Graph theory and molecular orbitals. Total p-electron energy of alternant hydrocarbons, hem. Phys. Lett. 17 (1972), 535–538.
11. Gutman, Selected properties of the Schultz molecular topological index, J. Chem. Inf. Comput. Sci. 34(1994) 1087–1089.
12. X. Li, I. Gutman, Mathematical aspects of Randi ´ c-type molecular structure descriptors, Univ. Kragujevac, 2006.
13. Gutman, B. Furtula, M. Petrovi ´ c, Terminal Wiener index, J. Math. Chem. 46 (2009) 522–531.
14. Gutman: Degree-based topological indices, Croat. Chem. Acta 86(2013), 351–361.
15. F. Harary, Graph Theory, Addison–Wesely, Reading, 1969.
16. Horvat, T. Pisanski, M. Randi ´ c, Terminal polynomials and star-like graphs, MATCH Commun. Math. Comput.Chem. 60 (2008) 493–512.
17. S. M. Hosamani, Ashwini index of a graph, Int. J. Industrial Mathematics, 8(4)(2016) 377–384.
18. S. M. Hosamani, An improved proof for the Wiener index when diam(G) _ 2, Math. Sci. Lett. 5(2)(2016) 1–2.
19. Ili´C, S. Klavžar, M. Milanovi´c: On distance-balanced graphs, Eur. J. Comb. 31(2010), 733–737.
20. J. Jerebic, S. Klavžar, D.F. Rall: Distance-balanced graphs, Ann. Comb. 12 (2008), 71–79

**JOURNAL OF ALGEBRAIC STATISTICS**
Volume 13, No. 2, 2022, p. 3338-3345
https://publishoa.com
ISSN: 1309-3452

21. K. Kutnar, A. Malniˇc, D. Marušiˇc, and S. Miklaviˇc: Distance-balanced graphs: symmetry conditions, Discrete Math., 306(2006), 1881–1894
22. S. Klavžar: A bird's eye view of the cut method and a survey of its applications in chemical graph theory, MATCH Commun. Math. Comput. Chem. 60(2008), 255–274
23. G. Liu, Z. Jia,W. Gao, (2018). Ontology Similarity Computing Based on Stochastic Primal Dual Coordinate Technique.Open j. math. sci., 2(1), 221-227.
24. Š. Miklaviˇc, P. Šparl: Distance-balanced graphs. Discrete Appl. Math. 244 (2018), 143–154
25. Plavsi´c, S. Nikoli´c, N. Trinajsti´c (1993). On the Harary index for the characterization of chemical graphs, J. Math. Chem12 (1993) 235–250.