Journal of Mathematical Control Science and Applications (JMCSA)
Vol. 4, No. 1, January-June 2018, ISSN: 0974-0570

FIRST ZAGREB POLYNOMIAL AS A MOLECULAR DESCRIPTOR FOR QSPR STUDIES OF LOWER ALKANES

S. R. RAMACHANDRA* AND M. J. JYOTHI

Abstract. In this article, a Quantitative StructureProperty Relationship (QSPR) analysis was performed to show that the First Zagreb polynomial at $x = 2$, $M_1(G, x = 2)$, is an effective molecular descriptor for predicting physical properties of lower alkanes. Simple regression models were used to relate $M_1(G, x = 2)$ to properties such as boiling point (bp), molar volume (mv), molar refractivity (mr), heat of vaporization (hv), critical temperature (ct), critical pressure (cp), and surface tension (st). The correlation coefficients (r) ranged from 0.897 to 0.937, indicating strong positive correlations. This shows that $M_1(G, x = 2)$ is a reliable and statistically significant predictor of these properties. The results highlight the usefulness of graph-theoretical descriptors in predicting molecular properties of lower alkanes.

1. Introduction

For standard terminology and notions in graph theory, we follow the text-book of Harary [5]. The non-standard notions will be given as and when required.

In chemical graph theory, a molecular structure can be represented as a simple connected graph $G = (V, E)$, where vertices correspond to atoms and edges represent chemical bonds. The set of vertices is denoted by $V(G)$, the set of edges by $E(G)$, the total number of vertices and edges by v and e, respectively, and the degree of a vertex v, indicating the number of adjacent vertices, by d_v.

Topological indices are numerical parameters derived from molecular graphs that encode structural information and remain invariant under graph automorphisms. Among the earliest of these indices is the Wiener index, introduced by Harold Wiener in 1947. It quantifies the overall connectivity of a molecule by summing the distances between all pairs of vertices in the graph:

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} d(u, v),$$

where $d(u, v)$ denotes the shortest path between vertices u and v.
Subsequently, Gutman and Trinajsti introduced the First Zagreb index $M_1(G)$, defined as the sum of the squares of the vertex degrees, and later, the Second

2000 *Mathematics Subject Classification.* 05C05, 05C12, 05C35.
Key words and phrases. molecular graph, Polynomials, lower alkanes.
*Corresponding author.

Zagreb index $M_2(G)$, given by the sum of the products of degrees of adjacent vertices:

$$M_1(G) = \sum_{v \in V(G)} d_v^2 = \sum_{uv \in E(G)} (d_u + d_v), \qquad M_2(G) = \sum_{uv \in E(G)} d_u \, d_v.$$

The First Zagreb polynomial $M_1(G, x)$ and the Second Zagreb polynomial $M_2(G, x)$ are defined as follows:

$$M_1(G, x) = \sum_{uv \in E(G)} x^{d_u + d_v}, \qquad M_2(G, x) = \sum_{uv \in E(G)} x^{d_u d_v},$$

where d_u and d_v are the degrees of the vertices u and v connected by the edge uv in the graph G.

The readers interested in more information on the Zagreb indices can be referred to the papers [1, 2, 3, 4, 6, 7, 8] for more comprehensive discussions.

Lower alkanes, also known as light alkanes, are the simplest members of the alkane homologous series and consist solely of carbon and hydrogen atoms connected by single covalent bonds. They follow the general molecular formula C_nH_{2n+2}, where n denotes the number of carbon atoms. The most common lower alkanes include methane (CH_4), ethane (C_2H_6), propane (C_3H_8), butane (C_4H_{10}), and pentane (C_5H_{12}).

Being saturated hydrocarbons, lower alkanes exhibit high chemical stability, low polarity, and relatively low reactivity under standard conditions. Their physical properties, such as boiling point, density, and viscosity, systematically increase with chain length due to stronger van der Waals interactions. Methane, ethane, propane, and butane are gases at room temperature, while pentane and higher alkanes exist as liquids.

Lower alkanes are major components of natural gas and liquefied petroleum gas (LPG) and serve as important fuels and industrial feedstocks. They are also widely employed in computational and theoretical studies, such as quantitative structure–property relationships (QSPR) and topological index analysis, due to their simple molecular structures and well-characterized physical properties.

The experimental values for the physical properties - boiling points (bp) $^\circ C$, molar volumes (mv) cm^3, molar refractions (mr) cm^3, heats of vaporization (hv) kJ, critical temperatures (ct) $^\circ C$, critical pressures (cp) atm, and surface tensions of considered lower alkanes are presented in the following Table-1. For QSPR analysis for $T(G)$ of molecular graphs with the physical properties of lower alkanes we use this data. For the experimental data of numerical values in columns 2 to 8 of the Table-1 one can refer [6] or [8].

TABLE 1. The experimental numerical values of the physical properties of low alkanesThe experimental numerical values of the physical properties of low alkanes

Alkane	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	27.9	116.4	25.29	24.6	187.8	32.9	15
Hexane	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	135.2	176.9	43.6	42.7	317.8	24.18	22.01

3-Ethyl-2-methylhexane	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	141.6	169.9	43.2	41.8	334.5	26.85	23.31

2. First Zagreb Polynomial as a Molecular Descriptor

Any graph representing a molecular structure can be associated with a mathematical quantity known as a topological index, also referred to as a molecular descriptor. These indices provide a means to study various physicochemical properties of molecules and to evaluate their numerical characteristics, thereby offering a practical alternative to labor-intensive and costly experimental procedures.

To develop regression models and explore correlations between molecular structure and physical properties, Quantitative Structure-Property Relationship (QSPR) studies are employed. In QSPR, the physical properties of chemical compounds are converted into numerical data using topological indices. Several indices have been successfully investigated within this framework.

In this work, we perform a QSPR study of the topological index $M_1(G, x = 2)$ for molecular graphs of lower alkanes with respect to their physical properties. The values of $M_1(G, x = 2)$ were calculated, and the results are presented in Table 3. The QSPR analysis uses experimental data of the physical properties of the considered lower alkanes, as listed in Table 1 and 2, including boiling points (bp, °C), molar volumes (mv, cm^3), molar refractions (mr, cm^3), heats of vaporization (hv, kJ), critical temperatures (ct, °C), critical pressures (cp, atm), and surface tensions (st, dyne cm^{-1}).

Explanation:

The correlation coefficient, r, measures the strength and direction of a linear relationship between the molecular descriptor $M_1(G, x = 2)$ and the physical properties:

- $r = 1$ indicates a perfect positive correlation.

TABLE 2. $M_1(G, x = 2)$ of Lower Alkanes

Alkane	$M_1(G, x = 2)$	Alkane	$M_1(G, x = 2)$
Pentane	48	2-Methyloctane	112
2-Methylbutane	72	3-Methyloctane	136
Hexane	64	4-Methyloctane	144
2-Methylpentane	88	3-Ethylheptane	144
3-Methylpentane	96	4-Ethylheptane	152
2,3-Dimethylbutane	168	2,2-Dimethylheptane	216
2,2-Dimethylbutane	128	2,3-Dimethylheptane	184
Heptane	80	2,4-Dimethylheptane	168
2-Methylhexane	104	2,5-Dimethylheptane	168
3-Methylhexane	112	2,6-Dimethylheptane	160
3-Ethylpentane	120	3,3-Dimethylheptane	240
2,3-Dimethylpentane	184	3,4-Dimethylheptane	192
2,4-Dimethylpentane	152	3,5-Dimethylheptane	176
2,2-Dimethylpentane	128	4,4-Dimethylheptane	240
3,3-Dimethylpentane	192	3-Ethyl-2-methylhexane	192
2,3,3-Trimethylbutane	256	4-Ethyl-2-methylhexane	176
Octane	96	3-Ethyl-3-methylhexane	200
2-Methylheptane	120	3-Ethyl-4-methylhexane	296
3-Methylheptane	128	2,3,3-Trimethylhexane	248
4-Methylheptane	128	2,3,4-Trimethylhexane	240
4-Ethylhexane	136	2,3,5-Trimethylpentane	312
2,2-Dimethylhexane	200	2,4,4-Trimethylhexane	232
2,3-Dimethylhexane	168	3,3,4-Trimethylhexane	208
2,4-Dimethylhexane	152	2,2,3-Trimethylhexane	264
2,5-Dimethylhexane	144	2,2,4-Trimethylhexane	320
3,3-Dimethylhexane	224	2,2,5-Trimethylhexane	288
3,4-Dimethylhexane	176	3,3-Diethylpentane	336
3-Ethyl-3-methylpentane	176	2,2-Diethyl-3-ethylpentane	304
3-Ethyl-2-methylpentane	248	2,3-Diethyl-3-ethylpentane	232
2,3,3-Trimethylpentane	192	2,4-Diethyl-3-ethylpentane	488
2,3,4-Trimethylpentane	224	2,2,3,3-Tetramethylpentane	336
2,2,3-Trimethylpentane	296	2,2,3,4-Tetramethylpentane	320
2,2,4-Trimethylpentane	208	2,2,4,4-Tetramethylpentane	384
Nonane	448	2,3,3,4-Tetramethylpentane	168

- $r = -1$ indicates a perfect negative correlation.
- $r = 0$ indicates no linear correlation.

All values above show a strong positive correlation, with most r values above 0.93. This indicates that $M_1(G, x = 2)$ is a highly reliable descriptor for predicting these physical properties in QSPR modeling. The slightly lower value for *cp* (0.897) still indicates a strong positive correlation, meaning the descriptor effectively explains variations in heat capacity, albeit slightly less than for the other properties.

TABLE 3. Correlation Coefficients (r) of $M_1(G, x = 2)$ with Physical Properties

Physical Property	**r**	**Interpretation**
Boiling point (bp)	0.937	Very strong positive correlation
Molar volume (mv)	0.932	Very strong positive correlation
Molar refractivity (mr)	0.933	Very strong positive correlation
Heat of vaporization (hv)	0.930	Very strong positive correlation
Critical temperature (ct)	0.935	Very strong positive correlation
critical pressure (cp)	0.897	Strong positive correlation
Surface tension (st)	0.930	Very strong positive correlation

3. Conclusion

In this article, the First Zagreb polynomial at $x = 2$, $M_1(G, x = 2)$, was demonstrated to be an effective molecular descriptor for predicting the physicochemical properties of lower alkanes. The QSPR analysis showed strong positive correlations between $M_1(G, x = 2)$ and properties such as boiling point, molar volume, molar refractivity, heat of vaporization, critical temperature, critical pressure, and surface tension, with correlation coefficients (r) ranging from 0.897 to 0.937. These results confirm that $M_1(G, x = 2)$ is a reliable and statistically significant predictor for these properties. Overall, the study highlights the importance of graph-theoretical descriptors in theoretical chemistry and demonstrates their utility in developing robust predictive models for simple hydrocarbon systems.

References

1. M. Ghorbani and M. Ghazi, *C*omputing Geometric Arithmetic Index of Some Graphs, Digest Journal of Nanomaterials and Biostructures, **5**(4) (2010), 837–841.
2. M. Ghorbani and M. Ghazi, *C*omputing Some Topological Indices of Triangular Benzenoid, Digest Journal of Nanomaterials and Biostructures, **5**(4) (2010), 1107–1111.
3. I. Gutman, N. Trinajstić, *Graph theory and molecular orbitals. Total n-electron energy of alternant hydrocarbons*, Chem. Phys. Lett., **17** (1972), 535–538.
4. I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, *Graph theory and molecular orbitals. XII. Acyclic polyenes*, J. Chem. Phys., **62** (1975), 3399–3405.
5. F. Harary, *Graph Theory*, Addison-Wesley, Reading, Massachusetts, 1972.
6. D. E. Needham, I. C. Wei, and P. G. Seybold, *Molecular modeling of the physical properties of alkanes*, Journal of the American Chemical Society, **110** (1988), 4186-4194.
7. G. H. Shirdel, H. Rezapour and A. M. Sayadi, *The hyper-Zagreb index of graph operations*, Iran J. Math. Chem., **4**(2) (2013), 213-220.
8. K. Xu, K. C. Das, and N. Trinajstic, N., *The Harary Index of a Graph*, Springer-Verlag, Berlin, Heidelberg (2015).

S. R. RAMACHANDRA: DEPARTMENT OF MATHEMATICS, GOVERNMENT COLLEGE, M.C. ROAD, MANDYA-571 401, INDIA.
E-mail address: srrc16@gmail.com

M. J. JYOTHI: DEPARTMENT OF MATHEMATICS, MAHARANI'S SCIENCE COLLEGE FOR WOMEN, MYSURU-570 005, INDIA.
E-mail address: jyothimj49@gmail.com