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A QSPR analysis for physical properties of lower alkanes involving Peripheral Wiener index

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Abstract

Establishing new relationships between the physical properties and the molecular structure of chemical compounds is very exciting. In this short paper, a QSPR analysis is carried for physical properties of lower alkanes involving Peripheral Wiener index, number of paths of length 3 and the number of vertices in molecular graphs and best multiple linear regression models are presented for boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of lower alkanes.

Keywords: Topological index, Peripheral Wiener index

2010 MSC: 05C12

1. Introduction

The text-book of Harary [2] has been referred for basic definitions and notions in graph theory. The non-standard notions will be given in this paper as and when required.

Let $G = (V, E)$ be a graph (finite, simple, connected and undirected). The order and size of G are $|V|$ and $|E|$, respectively. The distance between two vertices u and v in G, denoted by $d(u, v)$ is the number of edges in a shortest path (also called a graph geodesic) connecting u and v. The diameter of G, denoted by $d(G)$, is the length of the longest graph geodesic in G. The number of paths of length k in G is denoted by $p_k(G)$ or simply p_k. The eccentricity of a vertex v in G is the maximum distance between v and any other vertex in G. A vertex with maximum eccentricity in G is called a peripheral vertex in G. The vertices whose eccentricities are equal to the diameter of G are peripheral vertices of G. The set of all peripheral vertices of G is denoted by $PV(G)$. The symbol $\{u, v\}$ denotes an unordered pair of vertices in G.

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The topological indices are graph invariants that play a vital role in chemistry (see [1], [4]-[8], [12], [14]-[17]). They are theoretical molecular descriptors. The Wiener index is an important distance based topological indices defined for graphs, having numerous applications in Chemistry [16]. The Wiener index $W(G)$ of a graph G is defined as

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

The sum of distances between all unordered pairs of peripheral vertices in a graph G is called the Peripheral Wiener index (see [4], [9]-[11]) of G and is denoted by $PW(G)$:

$$PW(G) = \sum_{\{u,v\}\subset PV(G)} d(u,v).$$

The molecular graph of a chemical compound is a simple connected graph considering atoms of chemical compounds as vertices and the chemical bonds between them as edges. The number of vertices in a molecular graph G is denoted by $N(G)$ or simply N.

QSPR (Quantitative structure-property relationship) studies translates quantitative physical properties of chemical compounds into numerical data which helps to study correlation between properties of chemical compounds, their structure and simultaneously develop regression models. QSPR analysis for many topological indices has been carried out (*cf.* [3]) and the Peripheral Wiener index is one of the recent topological indices (defined in [10]) that is involved in the QSPR study carried out in this paper.

In this paper, by a QSPR analysis for physical properties of lower alkanes involving Peripheral Wiener index, number of paths of length three and the number of vertices in molecular graphs, we present best multiple linear regression models for boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of lower alkanes.

1.1. A QSPR analysis

We carry a correlation and multiple regression analysis for the physical properties-boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of lower alkanes with Peripheral Weiner index, number of paths of length 3 and the number of vertices in molecular graphs.

Table 1 gives the Peripheral Weiner index $PW(G)$, the number of paths p_3 of length three and the number of vertices N of molecular graphs and 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(st) $dyne\ cm^{-1}$ of considered alkanes. The values given in the columns 4 to 10 in the Table 1 are taken from Seybold et al. [14] and Needham et al. [12] (the same values can be found in [3, 17]).

Alkane	PW	p_3	N	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	4	2	5	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	8	2	5	27.9	116.4	25.29	24.6	187.8	32.9	15
Hexane	5	3	6	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	10	3	6	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	4	4	6	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	15	3	6	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	16	4	6	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	6	4	7	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	12	4	7	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	5	5	7	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	14	6	7	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	18	4	7	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	10	6	7	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	20	4	7	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	4	6	7	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	26	6	7	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	7	5	8	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	14	5	8	117.6	163.7	39.23	39.7	288	24.8	20.6

3-Methylheptane	6	6	8	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	6	6	8	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	14	7	8	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	21	5	8	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	12	7	8	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	12	6	8	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	24	5	8	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	5	7	8	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	5	8	8	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	22	8	8	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	12	9	8	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	18	8	8	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	32	5	8	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	10	9	8	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	20	8	8	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	8	6	9	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	16	6	9	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	7	7	9	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	7	7	9	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	16	8	9	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	6	8	9	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	24	6	9	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	14	8	9	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	14	7	9	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	14	7	9	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	28	6	9	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	6	8	9	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	6	9	9	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	6	8	9	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	6	8	9	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	25	9	9	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	26	8	9	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	14	10	9	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	14	10	9	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	21	9	9	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	21	7	9	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	38	6	9	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	12	10	9	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	12	10	9	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	24	8	9	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	12	8	9	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	5	11	9	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	24	12	9	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	34	10	9	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	22	12	9	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	36	10	9	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	18	12	9	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	32	10	9	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	48	6	9	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	20	12	9	141.6	169.9	43.2	41.8	334.5	26.85	23.31

Table 1. Peripheral Weiner Index, Number of paths of length 3 and Number of Vertices of molecular graphs, boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes

2. Regression models

Using Table 1, an initial study was carried out with a linear regression model

$$P = A + B(PW(G)),$$

where P =Physical property and $PW(G)$=Peripheral Wiener index and the correlation coefficent r is computed.

Physical Properties	r
bp	0.197251978
mv	0.346355015
mr	0.333426722
hv	0.142459634
ct	0.242716244
cp	-0.241588359
st	0.081503705

Table 2. Correlation coefficient r for the physical properties and the independent variable PW

The correlation coefficients r obtained in Table 2 for the physical properties were not good enough and we could not establish a satisfactory correlation between the Physical properties and Peripheral Wiener index of graphs of lower alkanes. The next approach involved multiple linear regression models with independent variables PW, p_3 and N.

Using Table 1, the correlation coefficient r and its square r^2 are computed and tabulated in Table 3 for the physical properties of lower alkanes and the explanatory (independent) variables PW, p_3 and N.

Physical Properties	r	r^2
bp	0.986832325	0.973838037
mv	0.999275529	0.998551584
mr	0.999951738	0.999903477
hv	0.974026826	0.948728258
ct	0.984031562	0.968318114
cp	0.977580064	0.955662782
st	0.957525168	0.916854447

Table 3. r and r^2 for the physical properties and the independent variables PW, p_3 and N

We have tested the following linear multiple regression model

$$P = A + B \cdot PW + C \cdot p_3 + D \cdot N,$$

where P = Physical property and obtained the following models:

$$bp = -90.04704 - 0.410913 \cdot PW + 0.787866 \cdot p_3 + 25.41022 \cdot N \tag{2.1}$$
$$mv = 29.84102 + 0.023342 \cdot PW - 1.67395 \cdot p_3 + 17.77645 \cdot N \tag{2.2}$$
$$mr = 1.633977 + 0.001304 \cdot PW - 0.124821 \cdot p_3 + 4.776364 \cdot N \tag{2.3}$$
$$hv = 1.830816 - 0.102587 \cdot PW - 0.157033 \cdot p_3 + 4.898461 \cdot N \tag{2.4}$$
$$ct = 73.49271 - 0.249444 \cdot PW + 4.387633 \cdot p_3 + 23.64618 \cdot N \tag{2.5}$$
$$cp = 47.86440 + 0.021757 \cdot PW + 0.722312 \cdot p_3 - 3.322539 \cdot N \tag{2.6}$$
$$st = 10.56800 - 0.042930 \cdot PW + 0.375619 \cdot p_3 + 1.029440 \cdot N \tag{2.7}$$

3. Conclusion

Table 3, reveals that the linear multiple regression models (2.1)-(2.7) are very useful tools in predicting the physical properties-boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of alkanes.

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