Section A-Research paper

A QSPR ANALYSIS FOR PHYSICAL PROPERTIES OF LOWER ALKANES USING FIRST STRESS INDEX

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Abstract: In this short paper, a QSPR analysis is carried for first stress index of molecular graphs and physical properties of lower alkanes and linear regression models are presented for boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions.

Keywords: Topological index, First Stress index, Lower Alkanes.

INTRODUCTION

The text-book of Harary [2] has been referred for terminologies 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). A shortest path between two vertices *u* and *v* in *G* is called a geodesic between *u* and *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 topological indices are graph invariants (theoretical molecular descriptors) that play an important role in chemistry (see [3, 5-10, 12]). There are many important degree/distance based topological indices defined for graphs having numerous applications in Chemistry [9] like Zagreb index, Wiener index, Harary index etc.

The concept of stress of a vertex in a network (graph) has been introduced by Shimbel [11] as a centrality measure in 1953. The concepts of stress number of a graph and stress regular graphs have been studied by K. Bhargava, N. N. Dattatreya and R. Rajendra in [1]. The stress of a vertex v in a graph G, denoted by $\mathrm{str}_G(v)$ or briefly by $\mathrm{str}(v)$, is the number of geodesics passing through it. The first stress index $S_1(G)$ is defined (See [4]) by

$$S_1(G) = \sum_{v \in V(G)} \mathrm{str}(v)^2 \qquad (1)$$

Quantitative structure-property relationship (QSPR) 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 can be found in literature. In this short paper, by a QSPR analysis for physical properties of lower alkanes involving first stress index of molecular graphs, we present best linear regression models for boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes.

A QSPR ANALYSIS

We carry a QSPR 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 first stress index of molecular graphs.

Table 1 gives the first stress index $S_1(G)$ 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 3 to 9 in the Table 1 are takenfrom Needham et al. [3] (the same values can be found in [10]).

Table 1.

Alkane	$S_1(G)$	bp $^{\circ}C$	mv cm^3	mr cm^3	hv kJ	ct $^{\circ}C$	cp atm	st $dynecm^{-1}$
Pentane	34	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	34	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	36	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	104	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	101	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	96	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	97	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	98	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	259	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	251	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	235	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	464	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	233	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	227	89.8	144.2	34.32	34.2	264.6	29.2	19.96

2,4-Dimethylpentane	243	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	219	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	225	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	560	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	545	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	512	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	497	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	464	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	505	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	482	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	497	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	530	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	461	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	464	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	449	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	432	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	382	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	490	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	598	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	467	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	1092	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	1068	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	1012	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	972	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	916	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	691	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	998	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	948	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	948	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	988	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	1044	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	908	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	892	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	932	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	870	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	852	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	892	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	820	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	836	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	878	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	918	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	974	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	846	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	868	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	924	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	884	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	828	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	772	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	822	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	796	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	828	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	814	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	718	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	904	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	822	141.6	169.9	43.2	41.8	334.5	26.85	23.31

Regression Models

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

$$P = A + B \cdot S_1(G),$$

Where P = Physical property and $S_1(G)$ = first stress index. The correlation coefficient r, its square r^2, standard error (*se*), *t*-value and *p*-value are computed and tabulated in Table 2 followed by linear regression models.

Table 2.

P	*r*	r^2	*se*	*T*	*P*
bp	0.9025	0.8145	(3.5951) (0.0051)	(16.5933) (17.1558)	(2.0057E-25)(3.2690E-26)
mv	0.9507	0.9038	(1.4293)(0.0020)	(91.4214)(25.0969)	(4.5297E-72)(8.6453E-36)
mr	0.9442	0.8916	(0.4618)(0.0006)	(64.5841)(23.4752)	(4.5066E-62)(4.8387E-34)
hv	0.9114	0.8308	(0.5887)(0.0008)	(49.7335)(18.1391)	(1.2648E-54)(1.4992E-27)
ct	0.8625	0.744	(5.1340)(0.0074)	(44.2971)(13.9550)	(2.3561E-51)(1.6752E-21)
cp	-0.8841	0.7817	(0.3266)(0.0004)	(94.32408)(-15.4932)	(5.6689E-73)(7.7881E-24)
st	0.7361	0.5419	(0.3497)(0.0004)	(52.5666)(8.6336)	(9.3618E-54)(2.7981E-12)

The linear regression models for boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes are as follows:

$$bp = 59.65619931 + 0.089084768 \cdot S_1(G) \quad (2)$$

$$mv = 130.6770037 + 0.051813343 \cdot S_1(G) \quad (3)$$

$$mr = 29.82607554 + 0.015658525 \cdot S_1(G) \quad (4)$$

$$hv = 29.27916439 + 0.015423992 \cdot S_1(G) \quad (5)$$

$$ct = 227.4248341 + 0.103481334 \cdot S_1(G) \quad (6)$$

$$cp = 30.80714628 - 0.007308723 \cdot S_1(G) \quad (7)$$

$$st = 18.38318834 + 0.004233504 \cdot S_1(G) \quad (8)$$

The values of r, r^2, *se*, *t* and *p* in Table 2 for the physical properties are good except for surface tensions which has $r^2 = 0.5419$. Hence the linear regression models (2)-(7) can be used as predictive tools.

CONCLUSION

Table 2, reveals that the linear regression models (2)-(7) are useful tools in predicting the physical properties-boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures and critical pressures of low alkanes. It shows that first stress index can be used as predictive means in QSPR researches.

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