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A QSPR Analysis for Square Root Stress-Sum Index

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Abstract: A QSPR analysis is carried for square root stress-sum 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 and critical temperatures.

Key Words: Topological index, square root stress-sum index, lower alkanes.

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§1. Introduction

Let $G = (V, E)$ be a graph (simple, finite, 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. For a glossary of graph theory terms, turn to the Harary's textbook [2]. As and when necessary, the non-standard notions will be provided in this document.

The topological indices are graph invariants (theoretical molecular descriptors) that play an important role in chemistry (see [3, 6, 7]). Many important degree or distance based topological indices can be found in literature for graphs having numerous applications in Chemistry [6] like Zagreb index, Wiener index, Harary index etc.

The quantitative structure-property relationship (QSPR) converts the quantitative physical characteristics of chemical compounds into numerical data, allowing researchers to investigate the relationships between these characteristics and the chemical compounds' structures while simultaneously creating regression models.

Shimbel [8] introduced the idea of stress of a vertex in a network (graph) as a centrality

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measure in 1953. K. Bhargava, N. N. Dattatreya, and R. Rajendra [1] have investigated the concepts of stress number of a graph and stress regular graphs.

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 square root stress-sum index $\mathcal{SRS}(G)$ of a simple graph G is defined (see [5]) by

$$\mathcal{SRS}(G) = \sum_{uv \in E(G)} \sqrt{\mathrm{str}(u) + \mathrm{str}(v)}. \tag{1}$$

In this paper, we present best linear regression models for boiling points, molar volumes, molar refractions, heats of vaporization and critical temperatures of low alkanes through a QSPR analysis for physical properties of lower alkanes with square root stress-sum index of molecular graph.

§2. 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 square root stress-sum index of molecular graphs.

Table 1 gives the square root stress-sum index $\mathcal{SRS}(G)$ 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 taken from Needham et al. [3] (the same values can be found in [7]).

Table 1. First Stress Index, boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes

Alkane	$\mathcal{SRS}(G)$	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	8.756	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	9.033	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	9.798	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	13.789	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	14.059	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	13.757	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	14.606	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	14.325	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	19.929	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	20.207	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	19.753	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	25.828	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	20.706	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	20.025	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	20.485	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	16.563	86.1	144.5	34.33	33	263	30	19.59

2,3,3-Trimethylbutane	20.975	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	27.179	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	27.468	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	26.902	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	26.772	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	32.034	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	27.955	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	27.055	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	27.191	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	27.757	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	27.137	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	26.618	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	26.109	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	26.288	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	26.607	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	28.244	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	29.101	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	27.338	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	35.537	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	35.839	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	35.181	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	34.963	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	33.801	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	32.034	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	36.327	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	35.259	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	35.265	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	35.483	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	36.141	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	35.303	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	34.599	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	34.825	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	35.052	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	33.729	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	34.102	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	33.963	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	33.434	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	35.742	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	35.971	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	36.629	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	35.344	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	34.895	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	35.560	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	35.605	130.6	177.2	43.66	40.8	309.1	23.79	21.17

3,3,4-Trimethylhexane	34.935	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	32.854	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	34.576	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	34.253	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	34.021	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	36.075	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	34.848	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	37.118	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	35.635	141.6	169.9	43.2	41.8	334.5	26.85	23.31

§3. **Regression Models**

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

$$P = A + B \cdot \mathcal{SRS}(G)$$

where P = Physical property and $\mathcal{SRS}(G)$ = square root stress-sum 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. r, r^2, se, t and p for the physical properties (P) and square root stress-sum index

P	r	r^2	se		t		p	
bp	0.9493	0.9013	(4.4601)	(0.1501)	(1.8548)	(24.7396)	(0.06801894400)	$(2.06038E-35)$
mv	0.9785	0.9576	(1.6138)	(0.0543)	(63.2757)	(38.9117)	$(1.73757E-61)$	$(1.01051E-47)$
mr	0.9856	0.9715	(0.4026)	(0.0135)	(51.9956)	(47.7961)	$(6.91797E-56)$	$(1.68657E-53)$
hv	0.9322	0.8690	(0.8810)	(0.0296)	(23.7143)	(21.0820)	$(2.63733E-34)$	$(2.78818E-31)$
ct	0.9294	0.8638	(6.3691)	(0.2144)	(25.8642)	(20.6137)	$(1.38438E-36)$	$(1.03014E-30)$
cp	−0.8803	0.7749	(0.5641)	(0.0189)	(61.2577)	(−15.1892)	$(1.46981E-60)$	$(2.19803E-23)$
st	0.7941	0.6306	(0.5619)	(0.0185)	(27.3738)	(10.4534)	$(4.82637E-37)$	$(1.78543E-15)$

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:

$$bp = 8.272946679 + 3.714688178 \cdot \mathcal{SRS}(G), \quad (2)$$

$$mv = 102.1199905 + 2.114125806 \cdot \mathcal{SRS}(G), \quad (3)$$

$$mr = 20.9376134 + 0.647931461 \cdot \mathcal{SRS}(G), \quad (4)$$

$$hv = 20.8936634 + 0.625307734 \cdot \mathcal{SRS}(G), \quad (5)$$

$$ct = 164.7337437 + 4.419939221 \cdot \mathcal{SRS}(G), \quad (6)$$

$$cp = 34.55588274 - 0.288452993 \cdot \mathcal{SRS}(G), \quad (7)$$

$$st = 15.38165627 + 0.193802145 \cdot \mathcal{SRS}(G). \quad (8)$$

The values of r,r^2, se, t and p in Table 2 for the physical properties are good except for

critical pressures and surface tensions. As a result the linear regression models (2) – (6) can be used as predictive tools.

§4. 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 and critical temperatures of low alkanes. It shows that square root stress-sum index can be used as predictive tool in QSPR researches.

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