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A QSPR Analysis for Stress-Sum Index

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Abstract: In this brief paper, the stress-sum index of molecular graphs and the physical characteristics of lower alkanes are analysed using QSPR, and linear regression models for boiling points, molar volumes, molar refractions, heats of vaporisation and critical temperatures are presented.

Key Words: Molecular graph, topological index, Stress sum index.

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§1. Introduction

Let $G = (V, E)$ be a graph (finite, simple, connected and undirected). A geodesic between two vertices u and v in G is a shortest path 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 definitions in graph theory, the textbook of Harary [2] has been cited. As and when necessary, the non-standard notions will be provided in this article.

The topological indices are graph invariants (theoretical molecular descriptors) that play an important role in chemistry (See [3-14]). There are many important degree/distance based topological indices defined for graphs having numerous applications in chemistry [13] like Zagreb index, Wiener index, Harary index etc.

The concept of stress of a vertex in a network (graph) has been introduced by Shimbel [15] 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

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passing through it. The stress-sum index $\mathcal{SS}(G)$ of a simple graph G is defined (see [6]) by

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

the quantitative structure-property relationship (QSPR) studies translate 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 stress-sum index of molecular graphs, we present best linear regression models for boiling points, molar volumes, molar refractions, heats of vaporization and critical temperatures of low alkanes.

§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 stress-sum index of molecular graphs.

Table 1 gives the stress-sum index $\mathcal{SS}(G)$ 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. [4] (the same values can be found in [14]).

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

Alkane	$\mathcal{SS}(G)$	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	20	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	21	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	24	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	40	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	41	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	40	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	44	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	42	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	70	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	71	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	69	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	104	93.5	143.5	34.28	35.2	267.6	28.6	20.44

(Table continues)

Alkane	$\mathcal{SS}(G)$	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
2,2-Dimethylpentane	74	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	70	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	72	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	59	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	75	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	112	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	113	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	110	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	109	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	104	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	116	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	110	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	111	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	114	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	112	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	108	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	105	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	108	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	105	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	117	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	129	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	111	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	168	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	169	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	175	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	163	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	156	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	138	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	172	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	164	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	164	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	166	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	170	135.2	180.9	43.93	42.8	306	23.7	20.83

(Table continues)

Alkane	$\mathcal{SS}(G)$	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
3,3-Dimethylheptane	166	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	160	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	162	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	164	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	154	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	157	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	158	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	153	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	167	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	169	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	173	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	165	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	161	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	165	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	167	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	163	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	152	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	160	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	159	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	155	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	170	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	156	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	176	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	166	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

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

where P = Physical property and $\mathcal{SS}(G)$ = 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 stress-sum index

P	r	r^2	se		t		p	
bp	0.9351	0.8744	(3.8323)	(0.0290)	(9.6718)	(21.6046)	$(2.4333E-14)$	$(6.6517E-32)$
mv	0.9716	0.9440	(1.4125)	(0.0106)	(83.6459)	(33.6272)	$(1.6608E-69)$	$(1.1145E-43)$
mr	0.9774	0.9553	(0.3838)	(0.0029)	(67.3975)	(37.8821)	$(2.702E-63)$	$(5.6412E-47)$
hv	0.9210	0.8484	(0.7220)	(0.0054)	(35.5945)	(19.3642)	$(3.0145E-45)$	$(3.7544E-29)$
ct	0.9155	0.8381	(5.2891)	(0.0400)	(37.6222)	(18.6270)	$(8.7678E-47)$	$(3.3851E-28)$
cp	−0.8672	0.7520	(0.4510)	(0.0034)	(71.6614)	(−14.257)	$(4.686E-65)$	$(5.6973E-22)$
st	0.7855	0.6170	(0.4216)	(0.00312)	(40.3860)	(10.1551)	$(2.9465E-47)$	$(5.7316E-15)$

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:

$$bp = 37.0657 + 0.6270 \cdot \mathcal{SS}(G) \quad (2)$$

$$mv = 118.1525 + 0.3597 \cdot \mathcal{SS}(G) \quad (3)$$

$$mr = 25.8679 + 0.1101 \cdot \mathcal{SS}(G) \quad (4)$$

$$hv = 25.6994 + 0.1058 \cdot \mathcal{SS}(G) \quad (5)$$

$$ct = 198.9881 + 0.7461 \cdot \mathcal{SS}(G) \quad (6)$$

$$cp = 32.32099 - 0.04870 \cdot \mathcal{SS}(G) \quad (7)$$

$$st = 17.0289 + 0.0317 \cdot \mathcal{SS}(G) \quad (8)$$

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 employed as predictive tools.

§4. Conclusion

The physical properties of low alkanes - boiling points, molar volumes, molar refractions, heats of vaporisation, and critical temperatures, can be predicted using the linear regression models (2)-(6), as shown in Table 2. It demonstrates that stress-sum index can be used as predictive means in QSPR researches.

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