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TOTAL STRESS AS A TOPOLOGICAL INDEX

H. MANGALA GOWRAMMA, P. SIVA KOTA REDDY, P. S. HEMAVATHI,
M. PAVITHRA, AND R. RAJENDRA

Abstract. In this article, we see the total stress of a graph as a topological index and obtain a formula for computing total stress index of trees. Also, we prove that total stress index of a graph G is zero iff G is complete. Further, a QSPR analysis has been carried to demonstrate that total stress index can be used as a predictive measure for physical properties of lower alkanes. Linear regression models involving total stress index have been presented for some physical properties of lower alkanes.

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Keywords and Phrases: Geodesic, Topological index, Total stress.

1. Introduction

For standard terminologies/notions in graphs the book by Harary [2] is followed. When necessary, this article will supply non-standard terms.

Let $G = (V, E)$ denote an undirected graph that is finite, simple and connected. A shortest path in G between two nodes x and y, is called a geodesic between x and y. A chemical compound's molecular graph is a simple connected graph where atoms of the chemical compound are considered as nodes and the chemical bonds between them are considered as edges.

Topological indices are nothing but theoretical molecular descriptors. They are graph invariants playing a vital role in Chemistry (see [6, 21, 22]). Many topological indices have been explored for graphs with considerable applications in Chemistry [21, 22] for instance, Wiener index, Zagreb index, Harary index etc.

Alfonso Shimbel [18] introduced the concept 'stress of a node' in a network in 1953 as a centrality measure. The stress of a node u in a graph G, denoted by $\mathrm{str}_G(u)$ (or simply $\mathrm{str}(u)$), if there is no possibility of confusion, is the number of geodesics passing through u. We denote the minimum stress among all the nodes of G by θ_G and the maximum stress amongst all the nodes of G by Θ_G. K. Bhargava et al. [1] have explored the concepts of total stress (stress number) of a graph G. The total stress of a graph G, denoted

[1]Corresponding author: pskreddy@jssstuniv.in; pskreddy@sjce.ac.in
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by $N_{\mathrm{str}}(G)$, is defined as

$$N_{\mathrm{str}}(G) = \sum_{u \in V} \mathrm{str}(u) \tag{1}$$

Raksha Poojary et al. [8,9] have studied the total stress of a graph G but by calling the stress of G. They have mainly studied the stresses of some standard graphs. They have determined the stress of a cut-node of G for the case when G has at most two cut-nodes. Within the families of all complete bipartite graphs of order n and all trees of order n, they have determined which graphs have the lowest and largest stress. They provide an intriguing formula and a technique to find stress using adjacency matrix, noting that it plays a significant role in determining the length of the shortest path and the distance between a given set of nodes.

Throughout this study, we refer to a graph as a simple connected graph. In section 2, we see Total stress as a topological index and obtain a formula for computing total stress index of a tree. Also, we prove that total stress index of a graph G is zero if and only if G is complete. Section 3 presents the results of a QSPR investigation of the physical properties of lower alkanes using the total stress index of molecular graphs, along with some excellent linear regression models for the physical properties.

2. Total stress as a molecular descriptor

A topological index, often referred to as a molecular descriptor, is a mathematical formula that may be applied to any graph that represents any molecular structure. One can evaluate mathematical values and look into some other physicochemical aspects of molecules using such a topological index. It is therefore a useful strategy for avoiding costly and time-consuming laboratory experiments. For stress based topological indices, we suggest the reader to refer the papers [3–5, 10–17, 19, 20].

The physical properties of chemical compounds are converted into numerical data via quantitative structure-property relationship (QSPR) investigations, which are then used to build regression models and investigate correlations between the physical attributes and the structure of the compounds. With QSPR, a number of topological indices have been examined.

Since isomorphic graphs have same total stress, the total stress is a graph invariant i.e., the total stress is a molecular descriptor(i.e., a topological index). We call total stress of a graph G as total stress index (TSI) of G. By the definition of total stress (see Eq.(1)), we have, for any graph G

$$\theta_G |V(G)| \leq N_{\mathrm{str}}(G) \leq \Theta_G |V(G)|.$$

This inequality gives the bounds for TSI of G. By counting the number of geodesics and the internal nodes in geodesics, we see that, for any graph G of diameter d, the TSI of G is given by

$$N_{\mathrm{str}}(G) = \sum_{i=1}^{d} f_i(i-1),$$

where f_i denotes the number of geodesics of length i in G (see [1, Proposition 2.6]). The following result is useful for computing TSI of tress.

Proposition 2.1. *For a tree T on n nodes, we have*

$$N_{str}(T) = \sum_{v \in I} \left[\sum_{1 \le i < j \le m} |C_i^v||C_j^v| \right], \tag{2}$$

where I is the set of all non-pendant internal nodes in T and the sets $C_1^v, \ldots, C_m^v$ denote the node sets in the components of $T - v$ for an internal node v of degree $m = m(v)$.

Proof. Since a pendant node in a tree T has zero stress, we concentrate on internal nodes and to compute the TSI. Let v be an internal node of T of degree $m = m(v)$. Let $C_1^v, \ldots, C_m^v$ be the components of the node deleted graph $T - v$. Using the fact that there is one and only one path between any two nodes in a tree, we have

$$\mathrm{str}(v) = \sum_{1 \le i < j \le m} |C_i^v||C_j^v|$$

(see [1, Proposition 3.2]). Hence by Eq.(1), we have

$$N_{\mathrm{str}}(T) = \sum_{v \in I} \left[\sum_{1 \le i < j \le m} |C_i^v||C_j^v| \right].$$

where I denotes the set of all non-pendant internal nodes in T. □

Theorem 2.2. *For a graph G, $N_{str}(G) = 0$ if and only if G is complete.*

Proof. Suppose that $N_{\mathrm{str}}(G) = 0$. Then by Eq.(1), $\mathrm{str}(v) = 0$ for all $v \in V(G)$. If $|V(G)| = 1$ or 2, then G is a complete graph as $G \cong K_1$ or K_2. Assume that $|V(G)| > 2$. Let u, v be any two distinct nodes in G. We claim that u, v are adjacent in G. For, if u, v are not adjacent in G, then there is a geodesic in G between u and v passing through at least one node, say w making $\mathrm{str}(w) \ge 1$, which a contradiction. Hence, u, v are adjacent in G. Therefore, G is complete.

Conversely, suppose that the graph G is complete. Then there is no geodesic of length ≥ 2 in G and consequently, $\mathrm{str}(v) = 0$ for all $v \in V(G)$. Then by Eq.(1), it follows that $N_{\mathrm{str}}(G) = 0$. □

3. A QSPR Analysis for TSI

In this section, we carry a QSPR analysis for TSI of molecular graphs with the physical properties of lower alkanes. To compute TSI of molecular graphs of low alkanes we have used Eq.(2).

The TSI N_{str} of molecular graphs and the experimental values for the physical properties of considered lower alkanes are presented in Table 1. For the experimental data of numerical values in columns 3 to 9 of the Table 1 one can refer [6] or [22].

Table 1. TSI N_{str} and the experimental numerical values of the physical properties of low alkanes

Alkane	N_{str}	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	10	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	8	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	6	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	20	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	17	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	16	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	13	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	14	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	35	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	31	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	29	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	44	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	25	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	25	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	27	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	23	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	21	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	56	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	51	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	48	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	47	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	44	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	43	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	42	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	43	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	46	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	39	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	40	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	39	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	36	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	32	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	38	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	38	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	37	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	84	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	78	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	74	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	72	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	68	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	61	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	68	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	66	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	66	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	68	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	72	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	62	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	62	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	64	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	60	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	60	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	62	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	56	140.6	173.1	43.27	43	327.2	25.66	23.22

3-Ethyl-4-methylhexane	58	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	56	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	58	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	62	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	54	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	56	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	60	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	56	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	52	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	52	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	50	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	52	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	54	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	46	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	46	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	52	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	48	141.6	169.9	43.2	41.8	334.5	26.85	23.31

Regression Models. An investigation was conducted using a linear regression model

$$Y = A + B \cdot N_{str}$$

where Y = Physical property and N_{str} = TSI, using Table 1. We have computed and tabulated the correlation coefficient r, its square r^2, standard error (se), t-value and p-value in Table 2.

Table 2. r,r^2, se, t and p for the physical properties (Y) and TSI

Y	r	r^2	se	t	p
bp	0.9087	0.8259	(4.3393) (0.0871)	(9.8099) (17.8287)	$(1.386E-14)$ $(3.919E-27)$
mv	0.9340	0.8724	(2.0505) (0.0411)	(59.3773) (21.4110)	$(1.143E-59)$ $(1.127E-31)$
mr	0.9160	0.8391	(0.7007) (0.0140)	(38.9367) (18.6961)	$(9.696E-48)$ $(2.747E-28)$
hv	0.9435	0.8903	(0.5905) (0.0118)	(43.9798) (23.3193)	$(3.754E-51)$ $(7.207E-34)$
ct	0.8377	0.7017	(6.9033) (0.1387)	(30.4995) (12.5556)	$(5.198E-41)$ $(2.884E-19)$
cp	−0.9349	0.8741	(0.3089) (0.0062)	(105.223) (−21.5770)	$(3.915E-76)$ $(7.170E-32)$
st	0.7117	0.5066	(0.4629) (0.0090)	(38.0398) (8.04289)	$(3.553E-45)$ $(3.001E-11)$

For the physical properties - boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes, the linear regression models are presented below:

$$bp = 42.5686 + 1.5544 \cdot N_{str} \tag{3}$$

$$mv = 121.7557 + 0.8821 \cdot N_{str} \tag{4}$$

$$mr = 27.2853 + 0.2632 \cdot N_{str} \tag{5}$$

$$hv = 25.9708 + 0.2767 \cdot N_{str} \tag{6}$$

$$ct = 210.5480 + 1.7415 \cdot N_{str} \tag{7}$$

$$cp = 32.5055 - 0.1339 \cdot N_{str} \tag{8}$$

$$st = 17.6122 + 0.0727 \cdot N_{str} \tag{9}$$

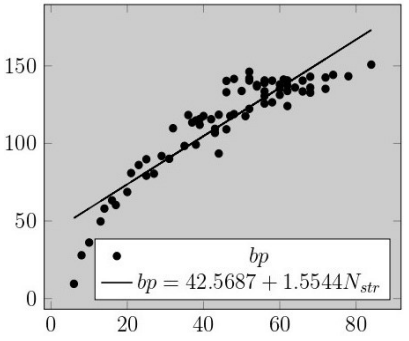

Figure 1. Model for bp

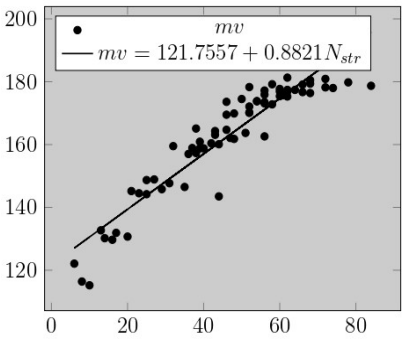

Figure 2. Model for mv

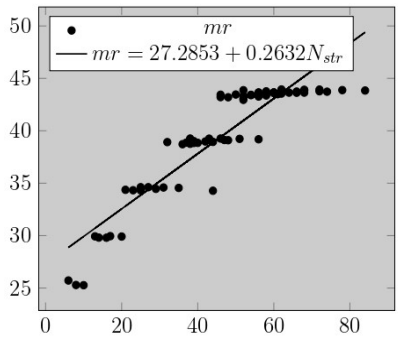

Figure 3. Model for mr

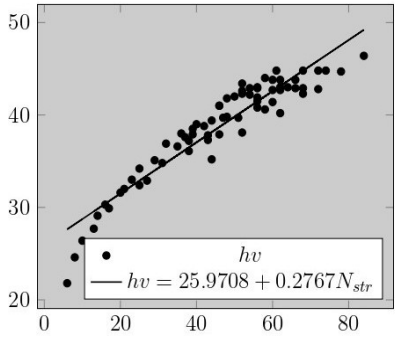

Figure 4. Model for hv

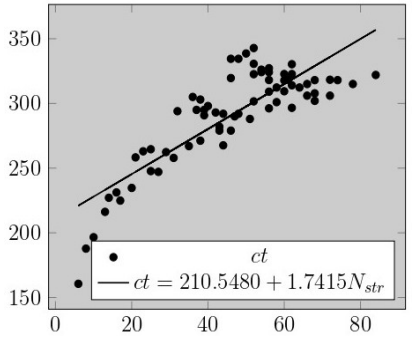

Figure 5. Model for ct

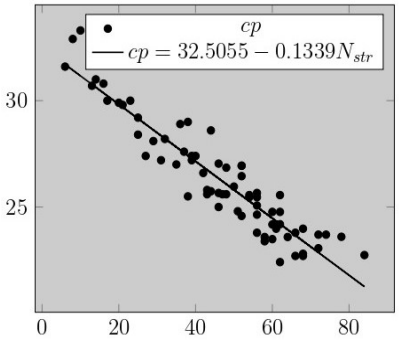

Figure 6. Model for cp

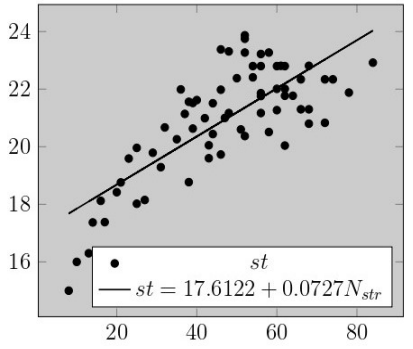

Figure 7. Model for st

For the physical properties the numerical values of r,r^2, se, t and p (shown in Table 2) are good except for the surface tension (for which $r^2 = 0.5066$). Therefore the linear regression models (3)-(8) can be used to make predictions.

4. Conclusion

From the Table 2, it follows that the linear regression models (3)-(8) are useful for predicting the physical properties of low alkanes except for the surface tension. This demonstrates that in QSPR investigations, the total stress index(TSI) may be employed as a predictive indicator.

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Department of Mathematics, Siddaganga Institute of Technology, Tumakuru-572103, INDIA, Affiliated to Visvesvaraya Technological University, Belagavi-590 018, INDIA
Email address: rgowrir@yahoo.com

Department of Mathematics, JSS Science and Technology University, Mysuru-570 006, INDIA
Email address: pskreddy@jssstuniv.in; pskreddy@sjce.ac.in

Department of Mathematics, Siddaganga Institute of Technology, Tumakuru-572103, INDIA, Affiliated to Visvesvaraya Technological University, Belagavi-590 018, INDIA
Email address: psh@sit.ac.in; hemavathisuresh@gmail.com

Department of Studies in Mathematics, Karnataka State Open University, Mysuru-570 006, INDIA
Email address: sampavi08@gmail.com

Department of Mathematics, Field Marshal K.M. Cariappa College (A constituent college of Mangalore University), Madikeri-571 201, INDIA
Email address: rrajendrar@gmail.com