

LÓPEZ-BONILLA INDEX FOR GRAPHS

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Abstract: Chemical reactivity or physical attributes are correlated with a chemical structure through a number known as the topological index of that structure. Several topological indices have been defined on graphs using degrees of vertices, for instance first and second Zagreb indices. In this paper, we introduce a new topological index of a graph called López-Bonilla index using tension on edges. Further, we establish some inequalities and compute López-Bonilla index for some standard graphs. Further, a QSPR analysis has been carried to demonstrate that

López-Bonilla index can be used as a predictive measure for physical properties of lower alkanes. Linear regression models involving López-Bonilla index have been presented for some physical properties of lower alkanes.

Keywords and Phrases: Geodesic, Tension on an edge, Topological index.

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1. Introduction

We recommend reading Harary's textbook [5] to the reader for standard terminology and concepts in graphs. This article will provide non-standard information when needed.

Throughout this paper, $G = (V, E)$ denotes a graph (finite, undirected and simple) and $V = V(G)$ and $E = E(G)$ denote vertex set and edge set of G , respectively. Two non-distinct edges in a graph are adjacent if they are incident on a common vertex. We consider that an edge in a graph is not adjacent to itself. A shortest path in G between two nodes x and y , is called a geodesic between x and y . We say that a graph geodesic P is passing through an edge e in G if e is an edge in P . The number of geodesics in G is denoted by f .

The stress of a vertex was introduced by A. Shimmel [29] in 1953. The stress of a vertex is a node centrality index. In a graph, a vertex's stress is nothing but the number of geodesics that pass through it [3, 29]. Using the stresses of vertices as a motivation, Rajendra et al. [18] have proposed some topological indices of for graphs. In a recent study, K. Bhargava, N. N. Dattatreya, and R. Rajendra [4] have explored the idea of tension on edge in a graph, drawing inspiration from the concept of stress on a vertex. For new stress/tension/degree based topological indices, we suggest the reader to refer the papers [1, 2, 6-13, 15-28, 30, 32, 33].

Let G be a graph and e be an edge in G . The tension on e , denoted by $\tau_G(e)$ or simply $\tau(e)$, is defined as the number of geodesics in G passing through e . Tension on an edge is always ≥ 1 . The total tension of G , denoted by $N_\tau(G)$, is defined as,

$$N_\tau(G) = \sum_{e \in E} \tau(e). \quad (1.1)$$

A graph G is said to be k -tension-regular if all its edges are of tension k .

The chemical structures of chemical compounds are represented by molecular graphs in molecular graph theory, and it is frequently discovered that there is a link between the molecular structure descriptor and the physico-chemical characteristics of the corresponding chemical compounds. Often referred to as topological indices, these molecular structure descriptors are numerical parameters derived from the molecular graphs that are inescapably invariant under automorphism. There-

fore, topological indices are a highly valuable tool for isomer discrimination. They have also demonstrated their relevance in nanotechnology, including the creation and development of novel pharmaceuticals, and quantitative structure-activity and structure-property relationships. In this paper, we introduce a new topological index of a graph called López-Bonilla index using tension on edges. Further, we establish some inequalities and compute López-Bonilla index for some standard graphs in section 2. Further, a QSPR analysis has been carried in section 3 to demonstrate that López-Bonilla index can be used as a predictive measure for physical properties of lower alkanes. Linear regression models involving López-Bonilla index have been presented for some physical properties of lower alkanes.

2. López-Bonilla Index

Definition 2.1. *The López-Bonilla index $\mathcal{L}_B$ of a graph G is defined by*

$$\mathcal{L}_B = |V(G)| + \sum_{e \in E(G)} \frac{1}{\tau(e)}. \quad (2.1)$$

Observation: From (2.1), it is clear that, for any graph G , $\mathcal{L}_B$ need not be an integer.

Proposition 2.1. *For any graph G , we have the following inequalities:*

$$|V| + \frac{|E|}{f} \leq \mathcal{L}_B \leq |V| + |E| \quad (2.2)$$

and

$$|V| + \frac{|E|}{N_\tau(G)} \leq \mathcal{L}_B. \quad (2.3)$$

Proof. Since $\tau(e) \geq 1$, $\frac{1}{\tau(e)} \leq 1$, $\forall e \in E(G)$, and from (2.1), we have

$$\mathcal{L}_B \leq |V| + |E|. \quad (2.4)$$

Since $\tau(e) \leq f$, $\frac{1}{f} \leq \frac{1}{\tau(e)}$, $\forall e \in E(G)$, and from the (2.1), we have

$$|V| + \frac{|E|}{f} \leq \mathcal{L}_B. \quad (2.5)$$

Combining (2.4) and (2.5), we get (2.2).

From (1.1), we have

$$\frac{1}{N_\tau(G)} = \frac{1}{\sum_{e \in E} \tau(e)} \leq \frac{1}{\tau(\alpha)} \quad (2.6)$$

where α is any edge in G . Inequality (2.6) gives

$$\begin{aligned} \sum_{\alpha \in E} \frac{1}{N_\tau(G)} &\leq \sum_{\alpha \in E} \frac{1}{\tau(\alpha)} \\ \implies |V| + \frac{|E|}{N_\tau(G)} &\leq \mathcal{L}_B. \end{aligned}$$

Proposition 2.2. *If G is a subgraph of a tree T , then*

$$\mathcal{L}_B \geq \mathcal{L}_B(T) + |V(G)| - |V(T)| - \sum_{e \in E(T) - E(G)} \frac{1}{\tau_T(e)}.$$

Proof. Let G be a subgraph of a tree T . Since, in a tree, between any two vertices there is one and only one path, $\tau_G(e) \leq \tau_T(e)$ for any edge e in G . So,

$$\frac{1}{\tau_G(e)} \geq \frac{1}{\tau_T(e)}, \forall e \in E(G).$$

Therefore, from (2.1),

$$\begin{aligned} \mathcal{L}_B &= |V(G)| + \sum_{e \in E(G)} \frac{1}{\tau_G(e)} \\ &\geq |V(G)| + \sum_{e \in E(G)} \frac{1}{\tau_T(e)} \\ &\geq |V(G)| - |V(T)| + |V(T)| + \sum_{e \in E(T)} \frac{1}{\tau_T(e)} - \sum_{e \in E(T) - E(G)} \frac{1}{\tau_T(e)} \\ &= \mathcal{L}_B(T) + |V(G)| - |V(T)| - \sum_{e \in E(T) - E(G)} \frac{1}{\tau_T(e)}. \end{aligned}$$

Proposition 2.3. *If G is k -tension regular, then*

$$\mathcal{L}_B = |V| + \frac{|E|}{k}. \quad (2.7)$$

Proof. If G is k -tension regular, then $\tau(e) = k$, $\forall e \in E(G)$ and so from (2.1), we have

$$\mathcal{L}_{\mathcal{B}} = |V| + \sum_{e \in E(G)} \frac{1}{k} = |V| + \frac{|E|}{k}.$$

Corollary 2.1.

1. For the complete graph K_n on n vertices, $\mathcal{L}_{\mathcal{B}}(K_n) = n + \binom{n}{2}$.
2. For the complete bipartite graph $K_{m,n}$, $\mathcal{L}_{\mathcal{B}}(K_{m,n}) = m + n + \frac{mn}{m+n-1}$.
3. For the cycle C_n on n vertices,

$$\mathcal{L}_{\mathcal{B}}(C_n) = \begin{cases} n + \frac{8n}{(n-1)(n+1)}, & \text{if } n \text{ is odd;} \\ n + \frac{8}{(n+2)}, & \text{if } n \text{ is even.} \end{cases}$$

Proof.

1. In the complete graph K_n , for any edge e , we have $\tau(e) = 1$. Therefore K_n is 1-tension regular graph. Hence by Proposition 2.3, we have

$$\mathcal{L}_{\mathcal{B}}(K_n) = |V(K_n)| + \frac{|E(K_n)|}{1} = n + \binom{n}{2}.$$

2. In the complete bipartite graph $K_{m,n}$, for any edge e , we have $\tau(e) = m+n-1$. Therefore $K_{m,n}$ is $(m+n-1)$ -tension regular graph. Hence by Proposition 2.3, we have

$$\mathcal{L}_{\mathcal{B}}(K_{m,n}) = (m+n) + \frac{|E(K_{m,n})|}{m+n-1} = m+n + \frac{mn}{m+n-1}.$$

3. Let e be any edge in the cycle graph C_n on n vertices. Then

$$\tau(e) = \begin{cases} \frac{(n-1)(n+1)}{8}, & \text{if } n \text{ is odd;} \\ \frac{n(n+2)}{8}, & \text{if } n \text{ is even.} \end{cases}$$

Therefore C_n is

$$\begin{cases} \frac{(n-1)(n+1)}{8}\text{-tension regular,} & \text{if } n \text{ is odd;} \\ \frac{n(n+2)}{8}\text{-tension regular,} & \text{if } n \text{ is even.} \end{cases}$$

Hence by Proposition 2.3, we have

$$\begin{aligned} \mathcal{L}_B(C_n) &= \begin{cases} n + \frac{|E(C_n)|}{\left\lceil \frac{(n-1)(n+1)}{8} \right\rceil}, & \text{if } n \text{ is odd;} \\ n + \frac{|E(C_n)|}{\left\lceil \frac{n(n+2)}{8} \right\rceil}, & \text{if } n \text{ is even.} \end{cases} \\ &= \begin{cases} n + \frac{8n}{(n-1)(n+1)}, & \text{if } n \text{ is odd;} \\ n + \frac{8}{(n+2)}, & \text{if } n \text{ is even.} \end{cases} \end{aligned}$$

Proposition 2.4. *If T is a tree with m edges $e_1, e_2, \dots, e_m$, then*

$$\mathcal{L}_B(T) = m + 1 + \sum_{i=1}^m \frac{1}{|V(C_{i1})||V(C_{i2})|}, \quad (2.8)$$

where C_{i1} and C_{i2} are the components of $T - e_i$, $1 \leq i \leq m$. Further, For a path P_n with n vertices,

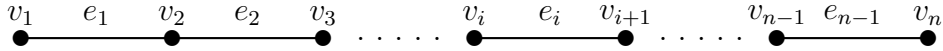
$$\mathcal{L}_B(P_n) = n + \sum_{i=1}^{n-1} \frac{1}{i(n-i)}.$$

Proof. For the edge e_i in T , let C_{i1} and C_{i2} be the components of $T - e_i$. Then

$$\tau(e_i) = |V(C_{i1})||V(C_{i2})|, \quad 1 \leq i \leq m.$$

Also, A tree with m edges has $m + 1$ vertices. Hence from (2.1), we have

$$\mathcal{L}_B(T) = m + 1 + \sum_{i=1}^m \frac{1}{|V(C_{i1})||V(C_{i2})|}.$$

Figure 1: The path P_n on n vertices.

A path P_n with n vertices, has $n-1$ edges $e_1, e_2, \dots, e_{n-1}$ (shown in the following figure). Clearly, $|V(C_{i1})| = i$ and $|V(C_{i2})| = n-i$ in $T - e_i$. Hence

$$\mathcal{L}_{\mathcal{B}}(P_n) = |V(P_n)| + \sum_{i=1}^{n-1} \frac{1}{|V(C_{i1})||V(C_{i2})|} = n + \sum_{i=1}^{n-1} \frac{1}{i(n-i)}.$$

Proposition 2.5. *Let W_n denote the wheel graph on $n \geq 5$ vertices. Then*

$$\mathcal{L}_{\mathcal{B}}(W_n) = n + \frac{n(n-1)}{3(n-3)}.$$

Proof. For the wheel graph W_n with $n \geq 5$, there are $(n-1)$ radial edges and $(n-1)$ peripheral edges. If e_p is a peripheral edge in W_n , then $\tau(e_p) = 3$ and if e_r is a radial edge in W_n , then $\tau(e_r) = n-3$. Hence from (2.1), we have

$$\begin{aligned} \mathcal{L}_{\mathcal{B}}(W_n) &= n + \sum_{\text{peripheral edges}} \frac{1}{\tau(e_p)} + \sum_{\text{radial edges}} \frac{1}{\tau(e_r)} \\ &= n + (n-1) \cdot \frac{1}{3} + (n-1) \cdot \frac{1}{(n-3)} \\ &= n + \frac{n(n-1)}{3(n-3)}. \end{aligned}$$

Proposition 2.6. *Let F_n denote the friendship graph on $2n+1$ vertices. Then*

$$\mathcal{L}_{\mathcal{B}}(F_n) = 2n+1 + \frac{n(2n+3)}{2n+1}.$$

Proof. In F_n , there are $3n$ edges, out of them $2n$ radial edges and n peripheral edges. If e_p is a peripheral edge in F_n , then $\tau(e) = 1$ and if e_r is a radial edge in F_n , then $\tau(e_r) = 2n+1$. Hence from (2.1), we have

$$\begin{aligned} \mathcal{L}_{\mathcal{B}}(F_n) &= 2n+1 + \sum_{\text{peripheral edges}} \frac{1}{\tau(e_p)} + \sum_{\text{radial edges}} \frac{1}{\tau(e_r)} \\ &= 2n+1 + n \cdot \frac{1}{1} + 2n \cdot \frac{1}{(2n+1)} \\ &= 2n+1 + \frac{n(2n+3)}{2n+1}. \end{aligned}$$

3. A QSPR Analysis for López-Bonilla index

In this section, we carry a QSPR analysis for López-Bonilla index of molecular graphs with the physical properties of lower alkanes. To compute López-Bonilla index of molecular graphs of low alkanes we have used Eq.(2.8).

The López-Bonilla index $\mathcal{L}_B$ 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 [14] or [34].

Table 1: López-Bonilla index $\mathcal{L}_B$ and the experimental numerical values of the physical properties of low alkanes

Alkane	$\mathcal{L}_B$	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	5.8333	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	5.9167	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	6.0000	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	6.7611	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	6.8361	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	6.8500	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	6.9250	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	6.9111	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	7.7000	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	7.7667	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	7.7833	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	7.8000	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	7.8500	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	7.8500	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	7.8333	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	7.8667	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	7.9167	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	8.6482	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	8.7077	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	8.7244	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	8.7286	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	8.7452	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	8.7839	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	8.7881	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	8.7839	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	8.7673	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	8.8048	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	8.8006	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	8.8048	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	8.8214	118.3	157	38.72	38	305	28.9	21.99

2,2,3-Trimethylpentane	8.8601	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	8.8435	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	8.8643	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	8.8476	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	9.6040	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	9.6575	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	9.6734	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	9.6790	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	9.6948	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	9.7004	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	9.7270	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	9.7325	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	9.7325	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	9.7270	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	9.7111	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	9.7484	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	9.7484	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	9.7429	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	9.7540	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	9.7540	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	9.7484	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	9.7698	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	9.6948	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	9.8020	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	9.7964	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	9.7806	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	9.8075	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	9.8020	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	9.7861	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	9.8020	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	9.8179	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	9.7857	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	9.8179	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	9.8234	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	9.8075	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	9.8714	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	9.8556	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	9.8500	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	9.7004	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

$$Y = A + B \cdot \mathcal{L}_B$$

where Y = Physical property and $\mathcal{L}_B$ = López-Bonilla index, 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 López-Bonilla index $\mathcal{L}_B$

Y	r	r^2	se		t		p	
bp	0.9675	0.9361	(7.7637)	(0.8669)	(-16.3265)	(31.3287)	(4.80622E - 25)	(9.67943E - 42)
mv	0.9828	0.9659	(3.1337)	(0.3499)	(8.7023)	(43.5315)	(1.30824E - 12)	(7.29016E - 51)
mr	0.9970	0.9941	(0.3980)	(0.0444)	(-5.7831)	(105.8042)	(2.10474E - 07)	(2.71348E - 76)
hv	0.9451	0.8931	(1.7212)	(0.1922)	(-0.9436)	(23.6637)	(0.348759585)	(2.99746E - 34)
ct	0.9590	0.9197	(10.5772)	(1.1810)	(0.0452)	(27.7033)	(0.964055368)	(2.04715E - 38)
cp	-0.8604	0.7402	(1.3109)	(0.1464)	(33.7738)	(-13.8176)	(8.46348E - 44)	(2.74697E - 21)
st	0.8738	0.7636	(1.1406)	(0.1258)	(6.4873)	(12.0748)	(1.46283E - 08)	(3.74342E - 18)

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 and their plots are presented below:

$$bp = -126.7535 + 27.1582 \cdot \mathcal{L}_B \quad (3.1)$$

$$mv = 27.2702 + 15.2317 \cdot \mathcal{L}_B \quad (3.2)$$

$$mr = -2.3017 + 4.7019 \cdot \mathcal{L}_B \quad (3.3)$$

$$hv = -1.6241 + 4.5478 \cdot \mathcal{L}_B \quad (3.4)$$

$$ct = 0.4785 + 32.7187 \cdot \mathcal{L}_B \quad (3.5)$$

$$cp = 44.2730 - 2.0225 \cdot \mathcal{L}_B \quad (3.6)$$

$$st = 7.3997 + 1.5186 \cdot \mathcal{L}_B \quad (3.7)$$

For the physical properties the numerical values of r, r^2, se, t and p (shown in Table 2) are very good. Therefore the linear regression models (3.1)-(3.7) can be used to make predictions for physical properties of low alkanes.

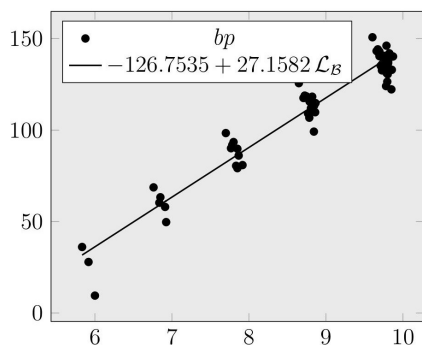


Figure 1: Model for bp

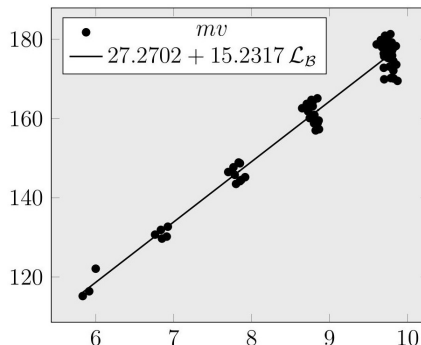
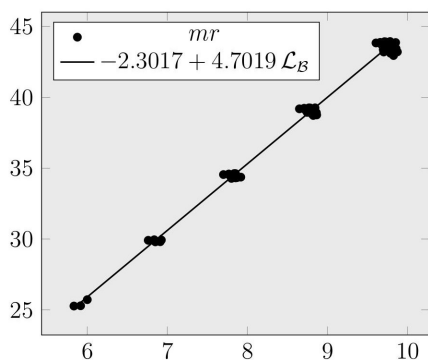
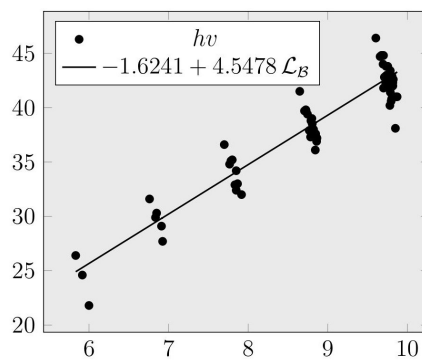
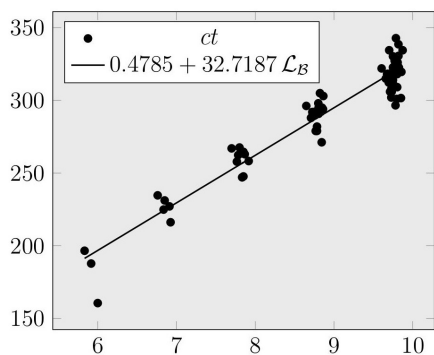
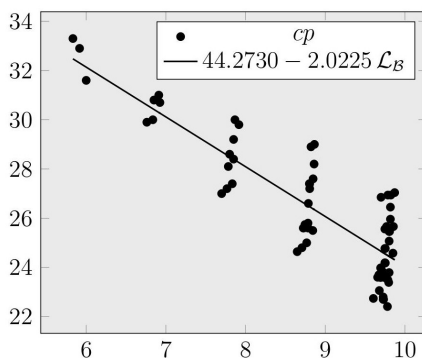
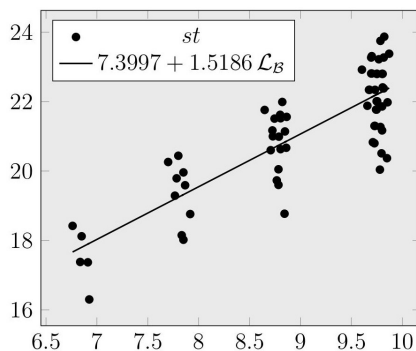


Figure 2: Model for mv

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

This indicates that the López-Bonilla index may be used as a predictive indicator in QSPR studies.

4. Conclusion

All graphs considered in this manuscript are simple. We have introduced a new

topological index of a graph called López-Bonilla index for graphs using tensions on edges and we obtained some results. We have demonstrated that in QSPR investigations the López-Bonilla index may be employed as a predictive indicator.

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