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CHELO INDEX FOR GRAPHS

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Abstract: It is exciting to study and establish relationships between the physical properties and the molecular structure of chemicals and there is a scope for defining new topological indices. This paper aims to introduce a new topological index for graphs called Chelo index. The Chelo index of a graph G is the sum of five times order of G and two times the number of geodesics of length 3 minus the number of geodesics between peripheral vertices. We compute Chelo index for some standard graphs and observe the correlation between some physical properties and Chelo index for low alkanes. Also, we establish a formulae for computing the number of

graph geodesics in a graph and the Chelo index using the adjacency matrix.

Keywords and Phrases: Adjacency matrix, Graph geodesic, Topological index.
2020 Mathematics Subject Classification: 05C12.

1. Introduction

We follow the text-book of Harary [4] for basic definitions and notions in graph theory. The non-standard will be given in this paper as and when required.

Let $G = (V, E)$ be a graph (finite, simple, connected and undirected). The order and size of G are respectively, $|V|$ and $|E|$. The distance between two vertices u and v in G, denoted by $d(u, v)$ is the number of edges in a shortest path (also called a graph geodesic) connecting them. The diameter of G, denoted by $d(G)$, is the length of the longest graph geodesic in G. The number of geodesics of length k in G is denoted by $\Gamma_k(G)$ or simply Γ_k. For two vertices u and v in G, $g(u, v)$ denotes the number of geodesics whose end vertices are u and v. The number of geodesics in G is denoted by $f(G)$ or simply f, and f_i denotes the number of geodesics of length i in G. Clearly, $f_1 = |E|$ and for a graph of diameter d, we have,

$$f(G) = \sum_{i=1}^{d} f_i \tag{1}$$

It is easy to see that

$$\sum_{\{u,v\}\subset V} g(u, v) = f(G) \tag{2}$$

The eccentricity of a vertex v in G is the maximum distance between v and any other vertex in G. A vertex with maximum eccentricity in G is called a peripheral vertex in G. So, vertices whose eccentricities are equal to $d(G)$ are peripheral vertices of G. The set of all peripheral vertices of G is denoted by $PV(G)$.

The topological indices play significant roles in the research related to drug development. There are many topological indices defined for graphs. Wiener index (see [16]) and Harary Index (see [17]) are some interesting topological indices defined based on graph distance. The Wiener index $W(G)$ of a connected graph G is defined to be the sum of distances between all vertex pairs in G. The Wiener index is substantially used in theoretical chemistry for the design of quantitative structure–property relations (mainly with physico-chemical properties) and quantitative structure–activity relations including biological activities of the respective chemical compounds. For new topological indices, we suggest the reader to refer the papers [7], [9-12].

Rajendra et al. [13] have recently introduced the concept of peripheral geodesic index. The peripheral geodesic index $Pg(G)$ of a graph G is defined as the number of geodesics between peripheral vertices of G i.e.,

$$Pg(G) = \sum_{\{u,v\} \subset PV(G)} g(u,v), \tag{3}$$

where $PV(G)$ is the set of all peripheral vertices of G. The following computations can be found in [13]: For a cycle C_n on n vertices,

$$Pg(C_n) = \begin{cases} \dfrac{n(n-1)}{2}, & \text{if } n \text{ is odd;} \\ \dfrac{n^2}{2}, & \text{if } n \text{ is even.} \end{cases} \tag{4}$$

For a complete graph K_n on n vertices,

$$Pg(K_n) = \frac{n(n-1)}{2} \tag{5}$$

For the complete bipartite graph $K_{m,n}$,

$$Pg(K_{m,n}) = \frac{1}{2}mn(m+n). \tag{6}$$

For a tree T with $k \geq 2$ pendant vertices,

$$Pg(T) = \frac{k(k-1)}{2} \tag{7}$$

From (7), it follows that, for a path P_n on $n \geq 2$ vertices, $Pg(P_n) = 1$; and for a star $K_{1,n}$ on $n+1$ vertices,

$$Pg(K_{1,n}) = \frac{n(n-1)}{2} \tag{8}$$

Let $Wd(n,m)$ denotes the windmill graph constructed for $n \geq 2$ and $m \geq 2$ by joining m copies of the complete graph K_n at a shared common vertex v. Then

$$Pg(Wd(n,m)) = \frac{m(n-1)(n-2)}{2} + \frac{m(m-1)(n-1)^2}{2} \tag{9}$$

Hence, for the friendship graph F_k on $2k+1$ vertices,

$$Pg(F_k) = k(2k-1) \tag{10}$$

For the wheel graph W_n on $n \geq 4$ vertices,

$$Pg(W_n) = \frac{n(n-1)}{2} \tag{11}$$

In section 2, we introduce a new topological index for graphs called Chelo index. In section 3, we compute Chelo index for some standard graphs. Further, we establish formulae for computing the number of graph geodesics in a graph and the Chelo index using the adjacency matrix. In section 4, a QSPR analysis has been carried for some physical properties of lower alkanes with Chelo indices of their molecular graphs.

2. Chelo Index - Definition and Example

Definition 2.1. *The Chelo index $Ch(G)$ of a graph $G = (V, E)$ is defined by*

$$Ch(G) = 5\,|V| + 2\,\Gamma_3 - \sum_{\{u,v\} \subset PV(G)} g(u, v) \tag{12}$$

Using (3), we can write

$$Ch(G) = 5\,|V| + 2\,\Gamma_3 - Pg(G) \tag{13}$$

That is, the Chelo index of G is the sum of five times order of G and two times the number of geodesics of length 3 minus the number of geodesics between peripheral vertices.

Observation. *If k denotes the number of peripheral vertices in a graph G, then we have $\binom{k}{2}$ pairs of peripheral vertices and there is at least one path between each pair and hence, we have, $\binom{k}{2} \leq Pg(G) \leq f(G)$ and hence*

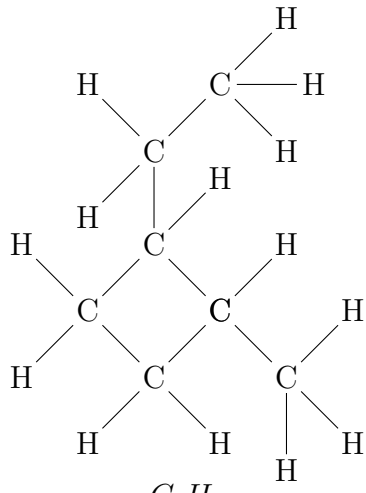
$$5\,|V| + 2\,\Gamma_3 - f(G) \leq Ch(G) \leq 5\,|V| + 2\,\mathcal{P}_3 - \binom{k}{2},$$

where $\mathcal{P}_3$ is the number of paths of length 3 in G.

Example 2.2. We compute the Chelo index of hydrogen-depleted molecular graph G of 1-Ethyl-2-methylcyclobutane C_7H_{14} (see Figure 1).

Here, $PV(G) = \{a, f, h\}$. We have $g(a, f) = 2$, $g(a, h) = 1$, and $g(f, h) = 1$. The number of geodesics of length 3 is $\Gamma_3 = 7$. The peripheral geodesic index of G is

$$Pg(G) = g(a, f) + g(a, h) + g(f, h) = 2 + 1 + 1 = 4.$$



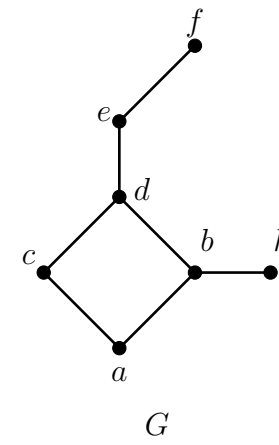


Figure 1: 1-Ethyl-2-methylcyclobutane C_7H_{14} and the corresponding hydrogen - depleted molecular graph G.

The Chelo index of G is

$$Ch(G) = 5|V| + 2T_3 - Pg(G) = 5 * 7 + 2 * 7 - 4 = 45.$$

3. Results

Proposition 3.1. *If G is a graph with $PV(G) = V(G)$, then*

$$Ch(G) = 5\,|V| + 2\,\Gamma_3 - f(G) \tag{14}$$

Proof. If $PV(G) = V(G)$, then $Pg(G) = f(G)$ and from (13), we have $Ch(G) = 5\,|V| + 2\,\Gamma_3 - f(G)$.

Proposition 3.2. *If G is a graph of diameter ≤ 2, then*

$$Ch(G) = 5\,|V| - Pg(G) \tag{15}$$

Proof. If G is a graph of diameter ≤ 2, then there is no geodesic of length 3 in G and so $\Gamma_3(K_n) = 0$. Hence, from (13), we have $Ch(G) = 5\,|V| - Pg(G)$.

Corollary 3.3.

1. *For a complete graph K_n on n vertices,*

$$Ch(K_n) = 5n - \frac{n(n-1)}{2} \tag{16}$$

2. *For the complete bipartite graph* $K_{m,n}$,

$$Ch(K_{m,n}) = 5(m+n) - \frac{1}{2}mn(m+n). \tag{17}$$

3. *For a star* $K_{1,n}$ *on* $n+1$ *vertices,*

$$Ch(K_{1,n}) = 5(n+1) - \frac{n(n-1)}{2} \tag{18}$$

4. *For the windmill graph* $Wd(n,m)$ *(constructed for* $n \geq 2$ *and* $m \geq 2$ *by joining* m *copies of the complete graph* K_n *at a shared common vertex),*

$$Ch(Wd(n,m)) = 5\left[m(n-1)+1\right] - \frac{m(n-1)(n-2)}{2} + \frac{m(m-1)(n-1)^2}{2}. \tag{19}$$

5. *For the friendship graph* F_k *on* $2k+1$ *vertices,*

$$Ch(F_k) = 5(2k+1) - k(2k-1). \tag{20}$$

6. *For the wheel graph* W_n *on* $n \geq 4$ *vertices,*

$$Ch(W_n) = 5n - \frac{n(n-1)}{2} \tag{21}$$

Proof. We have $d(K_n) = 1$, $d(K_{m,n}) = 2$, $d(K_{1,n}) = 2$, $d(Wd(n,m)) = 2$, $d(F_k) = 2$, and $d(W_n) = \begin{cases} 1, & \text{if } n = 4; \\ 2, & \text{if } n \geq 5. \end{cases}$
Hence, using (5), (6), (8), (9), (10) and (11) in (15), we get (16), (17), (18), (19), (20) and (21), respectively.

Proposition 3.4. *For a cycle* C_n *on* n *vertices,*

$$Ch(C_n) = \begin{cases} 12, & \text{if } n = 3; \\ 28, & \text{if } n = 4; \\ 35, & \text{if } n = 5; \\ 7n - \dfrac{n(n-1)}{2}, & \text{if } n > 5 \text{ and } n \text{ is odd}; \\ 7n - \dfrac{n^2}{2}, & \text{if } n > 5 \text{ and } n \text{ is even}. \end{cases} \tag{22}$$

Proof. We have

$$\Gamma_3(C_n) = \begin{cases} 0, & \text{if } n = 3, 4, 5; \\ n, & \text{otherwise.} \end{cases} \tag{23}$$

Now, using (4) and (23) in (15), we get (22).

Proposition 3.5. *For a tree T with n vertices and $k \geq 2$ pendant vertices,*

$$Ch(T) = 5n + 2\mathcal{P}_3 - \frac{k(k-1)}{2}, \tag{24}$$

where $\mathcal{P}_3$ is the number of paths of length 3 in T.

Proof. Since there is one and only one path between any two vertices in a tree, $\Gamma_3 = \mathcal{P}_3$. Hence, using (7) in (15), we get (24).

Corollary 3.6. *For a path P_n on $n \geq 2$ vertices, $Ch(P_n) = 7(n-1)$.*

Proof. There are 2 pendant vertices in P_n and the number of paths of length 3 is $\mathcal{P}_3 = n - 3$. Hence, from (24), we have

$$Ch(P_n) = 5n + 2(n-3) - 1 = 7(n-1).$$

3.1. Computation of Chelo index using adjacency matrix

Let G be a graph of diameter d with n vertices $v_1, \ldots, v_n$. Let $A = (a_{ij}^{(1)})$ be the adjacency matrix of the graph G, where

$$a_{ij}^{(1)} = \begin{cases} 1, & \text{if } v_i \sim v_j; \\ 0, & \text{otherwise.} \end{cases}$$

We consider the following powers of A: $A^2, \ldots, A^d$, where d is the diameter of G. We denote the (i,j)-th element of A^t $(2 \leq t \leq d)$, by $a_{ij}^{(t)}$, where

$$a_{ij}^{(t)} = \sum_{k=1}^{n} a_{ik}^{(t-1)} a_{kj}^{(1)}.$$

We know that $a_{ij}^{(t)}$ is the number of distinct edge sequences between v_i and v_j of length t. Let g_{ij} be the first non-zero entry in the sequence $a_{ij}^{(1)}, a_{ij}^{(2)}, \ldots, a_{ij}^{(d)}$. Clearly, g_{ij} is the the number of geodesics between v_i and v_j, i.e., $g(v_i, v_j) = g_{ij}$.

Let us define $\phi_{ij}^{(t)}$, $(1 \leq t \leq d)$ as follows:

$$\phi_{ij}^{(t)} = \begin{cases} 1, & \text{if } a_{ij}^{(1)} = a_{ij}^{(2)} = \cdots = a_{ij}^{(t-1)} = 0 \text{ and } a_{ij}^{(t)} \neq 0; \\ 0, & \text{otherwise.} \end{cases} \tag{25}$$

Then

$$g_{ij} = a_{ij}^{(1)} \cdot \phi_{ij}^{(1)} + a_{ij}^{(2)} \cdot \phi_{ij}^{(2)} + \cdots + a_{ij}^{(d)} \cdot \phi_{ij}^{(d)} = \sum_{t=1}^{d} a_{ij}^{(t)} \cdot \phi_{ij}^{(t)} \tag{26}$$

Suppose that G has k peripheral vertices. Without loss of generality we may assume that $v_1, \ldots, v_k$ are the peripheral vertices of G. Then,

$$Pg(G) = \sum_{1 \le i < j \le k} g_{ij} \tag{27}$$

Using (26) in (27), we get

$$Pg(G) = \sum_{1 \le i < j \le k} \sum_{t=1}^{d} a_{ij}^{(t)} \cdot \phi_{ij}^{(t)} \tag{28}$$

Also, the number of geodesics of length 3 in G is

$$\Gamma_3(G) = \sum_{1 \le i < j \le n} a_{ij}^{(3)} \cdot \phi_{ij}^{(3)} \tag{29}$$

Now, from (13), we have

$$Ch(G) = 5n + 2 \sum_{1 \le i < j \le n} a_{ij}^{(3)} \cdot \phi_{ij}^{(3)} - \sum_{1 \le i < j \le k} \sum_{t=1}^{d} a_{ij}^{(t)} \cdot \phi_{ij}^{(t)} \tag{30}$$

Thus, we have,

Theorem 3.7. *Let G be a (connected) graph of diameter d with $n \ge 2$ vertices $v_1, \ldots, v_n$ and k peripheral vertices $v_1, \ldots, v_k$. Let $A = (a_{ij}^{(1)})$ be the adjacency matrix of G and (i,j)-th element of A^t $(2 \le t \le d)$, is denoted by $a_{ij}^{(t)}$. Then*

$$Ch(G) = 5n + 2 \sum_{1 \le i < j \le n} a_{ij}^{(3)} \cdot \phi_{ij}^{(3)} - \sum_{1 \le i < j \le k} \sum_{t=1}^{d} a_{ij}^{(t)} \cdot \phi_{ij}^{(t)},$$

where $\phi_{ij}^{(t)}$, $(1 \le t \le d)$ is given by

$$\phi_{ij}^{(t)} = \begin{cases} 1, & \text{if } a_{ij}^{(1)} = a_{ij}^{(2)} = \cdots = a_{ij}^{(t-1)} = 0 \text{ and } a_{ij}^{(t)} \neq 0; \\ 0, & \text{otherwise.} \end{cases}$$

4. A QSPR Analysis

In this section, we carry a correlation and regression 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 Chelo indices of their molecular graphs. Table 1 gives the Chelo index $Ch(G)$ of molecular graphs and 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 Seybold et al. [14] and Needham et al. [8] (the same values can be found in [15, 17]).

Table 1: Chelo index of molecular graphs, boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of considered alkanes

Alkane	$Ch(G)$	$\frac{bp}{^{\circ}C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^{\circ}C}$	$\frac{cp}{atm}$	$\frac{st}{dyn\ cm^{-1}}$
Pentane	28	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	26	27.9	116.4	25.29	24.6	187.8	32.9	15
Hexane	35	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	33	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	37	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	30	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	32	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	42	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	40	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	44	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	37	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	44	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	37	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	46	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	37	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	49	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	47	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	51	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	51	117.7	162.1	39.12	39.7	290	25.6	21
4-Ethylhexane	51	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	44	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	51	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	49	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	44	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	53	112	160.9	39.01	37.9	290.8	27.2	20.63

3,4-Dimethylhexane	55	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	50	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	55	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	50	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	40	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	55	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	50	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	56	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	54	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	58	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	58	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	58	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	60	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	51	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	58	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	56	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	56	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	51	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	60	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	60	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	57	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	55	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	62	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	62	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	57	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	53	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	47	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	62	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	62	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	55	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	58	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	66	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	63	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	59	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	59	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	55	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	63	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	55	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	42	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	63	141.6	169.9	43.2	41.8	334.5	26.85	23.31

Regression Models

Using the Table 1, the correlation coefficient r and its square r^2 are computed

and tabulated in Table 2 for the physical properties and Chelo index.

Table 2: r and r^2 for Chelo Index

Physical Properties	r	r^2
bp	0.937177708	0.878302056
mv	0.833630383	0.694939615
mr	0.885502823	0.784115249
hv	0.911242566	0.830363014
ct	0.954199301	0.910496306
cp	0.670423775	0.449468038
st	0.957426302	0.916665124

We have tested the following linear regression model

$$P = A + B \cdot Ch$$

where P = Physical property and Ch = Chelo index, and obtained the following models:

$$\begin{aligned} bp &= -24.95707358 + 2.781403189 \cdot Ch \\ mv &= 90.41478652 + 1.435331744 \cdot Ch \\ mr &= 16.41176731 + 0.458782557 \cdot Ch \\ hv &= 15.25848718 + 0.468818224 \cdot Ch \\ ct &= 119.3706907 + 3.425882038 \cdot Ch \\ st &= 11.24998733 + 0.190913293 \cdot Ch \end{aligned}$$

5. Conclusion

Table 2 reveals that the Chelo index is an useful tool in predicting the physical properties - boiling points, heats of vaporization, critical temperatures, and surface tensions of low alkanes. Further, Chelo index has good correlations with the physical properties - molar volumes and molar refractions. Though Chelo index has a positive correlation ($r = 0.670423775$) with critical pressures, it may not be useful in predicting the critical pressures of low alkanes because $r^2 = 0.449468038$.

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