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Research Paper

Steiner k-Eccentric Connectivity Index: a Novel Steiner Distance-Based Index

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Abstract

Let G be a connected graph and S be a k element subset of the vertex set $V(G)$. The Steiner-k distance $d_G(S)$ between vertices of S is the minimum size among all connected subgraphs whose vertex set contains S. In this paper, we have defined the Steiner k-eccentric connectivity index and derived a closed formula for the same in case of some standard graphs. Also, we have used Steiner 3-eccentric connectivity index to predict values of boiling point of some primary and secondary amines, cross sectional area and molar refraction of alcohols. For each, regression model is developed and statistical analysis is conducted and these have ensured at least 97% accuracy.

1 Introduction

Chemical graph theory has risen to prominence in recent times due to its crucial role in the study of predicting molecular structure, chemical bond activity, Quantitative Structure Activity Relationships (QSAR), Quantitative Structure Property Relationships (QSPR), etc. [1–6]. Graph invariants known as topological indices are usually employed in such analyses and prediction of physical/chemical/ biological activity is conducted for hydrogen-depleted chemical structures, also known as molecular graphs [7], [8]. Today, there are thousands of indices in use since they are useful for forecasting a molecule's characteristics mathematically [7, 9–14].

Topological indices [6] are broadly classified into two classes, based on their own nature viz., whether they are degree-based or distance-based indices. Various degree-based indices are available in the literature, including the Balaban index [15], Harary index [16], Gutman index [17], Harmonic index [18], ABC index [19], Zagreb indices [20], Hyper Zagreb indices, to name a few. The oldest topological index known is the Wiener index [8, 21], infact the first one to be defined and is a distance-based index. Subsequently, many distance-based indices such as Mostar, Edge Wiener, Szeged, and Steiner Wiener indices [22, 23] were introduced, all of

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which have found numerous applications in applied chemistry, applied biology, pharmacology, environmental sciences [7, 16, 17, 19], etc. A novel, highly discriminating index namely, the eccentric connectivity index, was defined by Sharma et al. [24] that was based on both the degree of a vertex and its eccentricity and hence, distance. As it depended on both degree and distance, the eccentric connectivity index had way more applications than any index that was based on just degree or distance.

The Steiner distance, a natural extension of graph distance, was defined by Chartrand et al. [22]. The Steiner distance $d(S)$ for a set $S \subset V(G)$ of vertices is the smallest size of a connected subgraph of G whose vertex set contains S. Hence, when $|S| = 2$, $d(S)$ is exactly the usual distance between two vertices. Replacing distances with Steiner distances, many distance-based topological indices were generalized including the Wiener index [25–27].

As seen earlier, the topological indices have numerous applications in real world problems. The generalized indices based on Steiner distances are bound to have applications. The fact that these indices are hard to calculate, motivates researchers to obtain closed formulae, attainable bounds, and their dependencies on other parameters of a graph. It is a well-known fact that the "Steiner Problem" is an NP-complete and hence any parameter based on Steiner distance is also an NP problem. To harness the richness involved in the generalized distances in the form of Steiner distance and define topological indices based on these distances is a herculean task. In this paper, we have attempted one such, by defining the Steiner k-eccentric connectivity index and studying its properties in explaining/enhancing the predictability of physico/chemical parameters of molecular structures under consideration. Eccentric connectivity index has a proven track record in applied chemistry by determining boiling point, cross-sectional area and many other properties of different molecular graphs [24]. Apart from these, for many classes of graphs the eccentric connectivity index has been obtained in its closed form [28, 29]. Many bounds also have been established [30, 31]. Motivated by these applications and challenged by the generalization of distances to Steiner distance, introduction of a new topological index is worthwhile and necessary. The improvements in predicting the physical/chemical properties of some primary/secondary amines and alcohols justify the same.

2 Preliminaries

The eccentric connectivity index has been proved [24, 32] to provide a high degree of predictability of biological activities of diverse compounds. We now present a few foundational concepts and findings that support our primary results. Unless otherwise mentioned, all of the graphs taken into consideration here are simple, undirected and single-edged.

Definition 2.1. ([33]). The distance from a vertex u to a vertex v in a connected graph G is defined as the length of a shortest $u - v$ path in G.

Definition 2.2. ([33]). The eccentricity $e(v)$ of vertex v in a connected graph G is the distance to a vertex farthest from v. Thus $e(v) = max\{d(u, v) : u \in V\}$. The *radius*, $rad(G)$, is the minimum eccentricity among the vertices of G and *diameter*, $diam(G)$, is the maximum eccentricity.

Definition 2.3. ([24]). *The eccentric connectivity index* (ξ^c) of a graph G is defined as the sum of the products of degree and eccentricity of all vertices of graph G.

$$\xi^c(G) = \sum_{i \in V(G)} d_i e_i,$$

where d_i and e_i are the degree and eccentricity of vertex i in a graph G.

Definition 2.4. ([25]). The Steiner distance $d(S)$ for a subset S of $V(G)$, is the minimum size (the number of edges) of a connected subgraph whose vertex set contains S.

Definition 2.5. ([25]). The Steiner k-eccentricity $e_k(v)$ of a vertex v of G is defined by $e_k(v) = max\{d(S)/S \subseteq V(G), |S| = k\}$.

Definition 2.6. ([25]). The Steiner k-radius of G is $srad_k(G) = min\{e_k(v)/v \in V(G)\}$.

Definition 2.7. ([25]). The Steiner k-diameter of G is $sdiam_k(G) = max\{e_k(v)/v \in V(G)\}$.

3 Results

As discussed above, Steiner distance is an important concept helpful in chemical graph theory. To harness the richness of this generalized distance, we first define a new, novel, more discriminating topological index that depends on Steiner k-eccentricity of a graph G.

Definition 3.1. The Steiner k-eccentric connectivity index ξ_k^c of a graph G is the sum of the products of degree of a vertex i and Steiner k-eccentricity of i in the graph G.

Thus,

$$\xi_k^c(G) = \sum_{i \in V(G)} d_i e_{k_i}. \tag{1}$$

Note: The eccentric connectivity index can be obtained from Steiner k-eccentric connectivity index by substituting $k = 2$. For any other $k \geq 3$, we observe that $\xi^c(G) \leq \xi_k^c(G)$ for any connected graph G.

We now derive closed-form expression for the Steiner k-eccentric connectivity index in the case of some special classes of graphs, as the general problem of determining the Steiner k-eccentricity itself is an open problem. We first give a result on complete graphs.

Proposition 3.2. *The Steiner k-eccentric connectivity index of a complete graph K_n is given by $\xi_k^c(K_n) = n(n-1)(k-1)$.*

Proof. For complete graphs K_n, we know that, $d(v) = n-1$, $e_k(v) = k-1$, $\forall v \in V(K_n)$. Hence,

$$\xi_k^c(K_n) = \sum_{i \in V(G)} d_i e_{k_i} = n(n-1)(k-1).$$

■

Proposition 3.3. *The Steiner k-eccentric connectivity index of a star graph S_n, $\forall n \geq 3$, is given by*

$$\xi_k^c(S_n) = \begin{cases} (2k-1)(n-1), & \text{if} \quad 2 \leq k \leq n-1, \\ 2(k-1)(n-1), & \text{if} \quad k = n. \end{cases}$$

Proof. In a star graph S_n, if we denote the central vertex as v_0 and the rest $n-1$ as v, then $d(v_0) = n-1$ and $d(v) = 1$.
Case(i) If $2 \leq k \leq n-1$, we see that, $e_k(v_0) = k-1$, $e_k(v) = k$, then

$$\xi_k^c(S_n) = (n-1)(k-1) + (n-1)(k) = (2k-1)(n-1).$$

Case(ii) For $k = n$, we observe that $e_k(v_0) = e_k(v) = k-1$, then

$$\xi_k^c(S_n) = (n-1)(k-1) + (n-1)(k-1) = 2(k-1)(n-1).$$

■

Proposition 3.4. *The Steiner k-eccentric connectivity index of a complete bipartite graph is given by*

$$\xi_k^c(K_{a,b}) = \begin{cases} 2abk, & \text{if } 1 \leq k \leq a, \\ (2k-1)ab, & \text{if } a < k \leq b, \\ 2(k-1)ab, & \text{if } b < k \leq a+b. \end{cases}$$

Proof. For $K_{a,b}$, we can partition the vertex set into U and W, so that $d(u_i) = a$.
Case(i) For $1 \leq k \leq a$, the Steiner k-eccentricity is given by $e_k(u_i) = e_k(w_i) = k$. Hence

$$\xi_k^c(K_{a,b}) = \sum_{i \in U} d_i e_{i_k} + \sum_{i \in W} d_i e_{i_k} = (a)bk + (b)ak = 2abk.$$

Case(ii) For $a < k \leq b$, we see that, $e_k(u_i) = k-1$, $e_k(w_i) = k$, giving

$$\xi_k^c(K_{a,b}) = \sum_{i \in U} d_i e_{i_k} + \sum_{i \in W} d_i e_{i_k} = a[b(k-1)] + b[ak] = ab(2k-1).$$

Case(iii) For $b < k \leq a+b$, we observe that, $e_k(u_i) = e_k(w_i) = k-1$. Thus,

$$\xi_k^c(K_{a,b}) = \sum_{i \in U} d_i e_{i_k} + \sum_{i \in W} d_i e_{i_k} = a[b(k-1)] + b[a(k-1)] = 2ab(k-1).$$

■

Proposition 3.5. *The Steiner k-eccentric connectivity index of a wheel graph W_n, $\forall n \geq 4$, is given by*

$$\xi_k^c(W_n) = \begin{cases} (4k-1)(n-1), & \text{if } k \leq n-3, \\ 4(k-1)(n-1), & \text{if } \quad k > n-3. \end{cases}$$

Proof. For a wheel graph, we know that the degree of the central vertex, say, $v_0 = n-1$ and degree 3 for remaining vertices, say v. We observe that for $k \leq n-3$, the k- eccentricity is given as $e_k(v_0) = k-1$ and $e_k(v) = k$. Thus,

$$\xi_k^c(W_n) = (n-1)3(k) + (n-1)(k-1) = (4k-1)(n-1).$$

For $k > n-3$, we see that $e_k(v_0) = e_k(v) = k-1$. Giving

$$\xi_k^c(W_n) = (n-1)3(k-1) + 1(n-1)(k-1) = 4(k-1)(n-1).$$

■

Proposition 3.6. *The Steiner k-eccentric connectivity index of a path P_n is given by $\xi_k^c(P_n) = 2(n-1)^2$, for $k > 2$.*

Proof. For paths P_n, it is clear that the degree of end vertices is one and the remaining vertices are two. And k-eccentricity is $e_k(v) = n-1$, $\forall v \in G$, $k > 2$. Thus,

$$\xi_k^c(P_n) = \sum_{i \in V(G)} d_i e_{i_k} = 2(n-1) + (n-2)(2)(n-1) = 2(n-1)^2.$$

■

Note: For a path graph P_n with $k \geq 3$, $e_k(v)$ depends only on n, as the maximum of Steiner distance is contributed by end vertices having distance $n-1$. In other words, the value of $e_k(v)$ is determined exclusively by the length of path.

Proposition 3.7. *The Steiner k-eccentric connectivity index for an even cycle is given by*

$$\xi_k^c(C_n) = \begin{cases} 2n(\frac{n}{2}+k-2), & \text{if } 2 \leq k \leq \frac{n}{2}-1, \\ 2n(n-2), & \text{if } \frac{n}{2} \leq k \leq n-1, \\ 2n(n-1), & \text{if } k = n. \end{cases}$$

Proof. Clearly, the degree of each vertex in a cycle is two and each vertex has the same eccentricity, making it a self-centered graph. For $k = 2$, we know that the Steiner 2-eccentricity of a vertex v, or just the eccentricity is diameter of an even cycle which is equal to $\frac{n}{2}$. Hence, cover $\frac{n}{2}+1$ vertices. For $2 < k \leq \frac{n}{2}-1$, maximum distance to cover these k vertices is $\frac{n}{2}+k-2$. For the case $\frac{n}{2} \leq k \leq n-1$, the maximum Steiner distance required to cover these k number of vertices is $n-2$. Therefore, Steiner k-eccentricity of every vertex for this case is $n-2$. For $k = n$, the maximum Steiner distance required to cover k number of vertices is n as it forms a path. Therefore, the Steiner k-eccentricity of vertices in an even cycle is given by

$$e_k(C_n) = \begin{cases} \frac{n}{2}+k-2, & \text{if } 2 \leq k \leq \frac{n}{2}-1, \\ (n-2), & \text{if } \frac{n}{2} \leq k \leq n-1', \\ (n-1), & \text{if } k = n. \end{cases}$$

Therefore, Steiner k-eccentric connectivity index for even cycles is obtained by multiplying Steiner k-eccentricity and $2n$ (degree 2 and such n number of vertices are there).

$$\xi_k^c(C_n) = \begin{cases} 2n(\frac{n}{2}+k-2), & \text{if } 2 \leq k \leq \frac{n}{2}-1, \\ 2n(n-2), & \text{if } \frac{n}{2} \leq k \leq n-1, \\ 2n(n-1), & \text{if } k = n. \end{cases}$$

■

Proposition 3.8. *The Steiner k-eccentric connectivity index for an odd cycle, for* $\frac{n-1}{2} \leq k \leq n$ *is given as follows:*

$$\xi_k^c(C_n) = \begin{cases} 2n(n-3), & \text{if } k = \frac{n-1}{2}, \\ 2n(n-2), & \text{if } \frac{n+1}{2} \leq k \leq n-1, \\ 2n(n-1), & \text{if } k = n. \end{cases}$$

Proof. Proof is similar to the above result. ■

4 Quantitative structure activity relation (QSAR) study of some chemical compounds using Steiner 3-eccentric connectivity index

It is a well-known fact that, to develop QSAR models with good predictive ability appropriate molecular descriptors have to be chosen. A molecular descriptor aims to mathematically characterize a molecular structure as completely as possible. The most widely used molecular descriptors are graph invariants due to their formulations from graph theory and are more

commonly referred to as Topological Indices (TIs) as they describe the topology of a molecule. In this section, we give an application of the newly introduced TI, the Steiner k-eccentric connectivity index in the previous sections, in determining many physico chemical activities to aid QSAR studies. We have selected various datasets encompassing physical and biological characteristics to assess the practicality of the Steiner k-eccentric connectivity index. Specifically, we are focusing on $k = 3$ to develop for QSAR models. Among them are the following:
1. A group of 21 primary and 13 secondary amines along with their boiling points (BPs) as given in [24] Tables 1 and 3.
2. A group of 14 straight and branched chain alcohols along with their cross-sectional areas (Table 5).
3. A group of 11 straight and branched chain alcohols along with their molar refraction values (Table 7).
For all of the datasets 1-3, values for the Steiner 3-eccentric connectivity index and the eccentric connectivity index were determined and the resulting data was then subjected to non-linear regression analyses. We determined appropriate equations, correlation coefficients, average errors (derived from the percentage error of each compound in a dataset), root mean square (RMS) errors and their comparison plots, which are listed below in Tables 1 to 7 and Figures 1 to 3.

Table 1: Comparison of the boiling points of primary amines using Steiner 3-eccentric connectivity index and eccentric connectivity index.

				Predicted BP $^{\circ}C$	
Compound	ξ_3^c	ξ^c	expt	ξ_3^c	ξ^c
Primary amines					
n-propylamine	18	18	49	50.98	58.68
2-aminopropane	11	9	33	37.09	31.11
2-amino2-methylpropane	12	12	46	39.13	40.68
2-aminobutane	27	19	63	67.44	61.54
2-methylpropylamine	27	19	69	67.44	61.54
n-butylamine	32	24	77	75.93	75.25
2-amino2-methylbutane	34	24	78	79.20	75.25
2-aminopentane	43	31	92	93.07	92.88
2-methylbutylamine	43	29	96	93.07	88.02
3-methylbutylamine	43	31	96	93.07	92.88
n-pentylamine	50	38	104	102.95	108.78
4-methylpentylamine	63	45	125	119.38	123.09
n-hexylamine	72	54	130	129.43	139.31
3-methylpentylamine	63	45	114	119.38	123.09
4-aminoheptane	87	61	139	144.07	150.37
2-aminoheptane	87	65	142	144.07	156.11
n-heptylamine	98	74	155	153.38	167.63
n-octylamine	128	96	180	174,30	188.47
n-nonylamine	180	122	201	204.53	202.26
2aminoundecane	223	168	237	235.98	206.52
3-aminopentane	43	29	91	93.07	88.02

Table 2: Regression statistics for boiling point of primary amines.

Properties	BP of primary amines from ξ_3^c
Multiple R	0.99766
R^2	0.99532
Adjusted R^2	0.99480
CC(%)	99.76608
Avg error (%)	3.586394
RMS error(%)	5.119899
F	213.00250

The regression equation for BP of primary amines is

$$BP(Primary \quad amines) = 13.19 + 2.293\xi_3 - 1.115 \times 10^{-2}\xi_3^2 + 2.397 \times 10^{-5}\xi_3^3. \qquad (2)$$

Table 3: Comparison for boiling points of secondary amines using Steiner 3-eccentric connectivity index and eccentric connectivity index.

				Predicted BP	$^\circ C$
Compound	ξ_3^c	ξ^c	expt	ξ_3^c	ξ^c
Secondary amines					
n-methylethylamine	18	18	36	38.19	44.08
n-methyl1-methyl ethylamine	27	19	50	51.83	46.32
diethylamine	32	24	56	59	57.19
n-methyl 1-methylpropylamine	43	29	78.5	73.81	67.54
n-ethyl propylamine	50	38	80.5	82.58	84.95
bis (1-methylethyl)amine	52	38	84	85	84.95
n-methyl butylamine	50	38	90.5	82.58	84.95
n-methyl 1-methyl butylamine	63	45	105	97.66	97.44
dipropylamine	98	74	109.5	131.73	112.24
bis(2-methylpropyl)amine	100	76	139	133.45	142.9
dibutylamine	128	96	159	155.62	164.79
bis(3-methylbutyl)amine	164	126	187.5	181.32	188.67
dipentylamine	200	150	205	207.7	201.75

Table 4: Regression statistics for boiling point of secondary amines.

Properties	BP of secondary amines from ξ_3^c
Multiple R	0.98868
R^2	0.97749
Adjusted R^2	0.97299
CC(%)	98.86833
Avg error (%)	5.51162
RMS error(%)	7.30550
F	43.43429

The regression equation for BP of secondary amines is

$$BP(Secondary \quad amines) = 7.83 + 1.808\xi_3 - 6.987 \times 10^{-3}\xi_3^2 + 1.473 \times 10^{-5}\xi_3^3. \qquad (3)$$

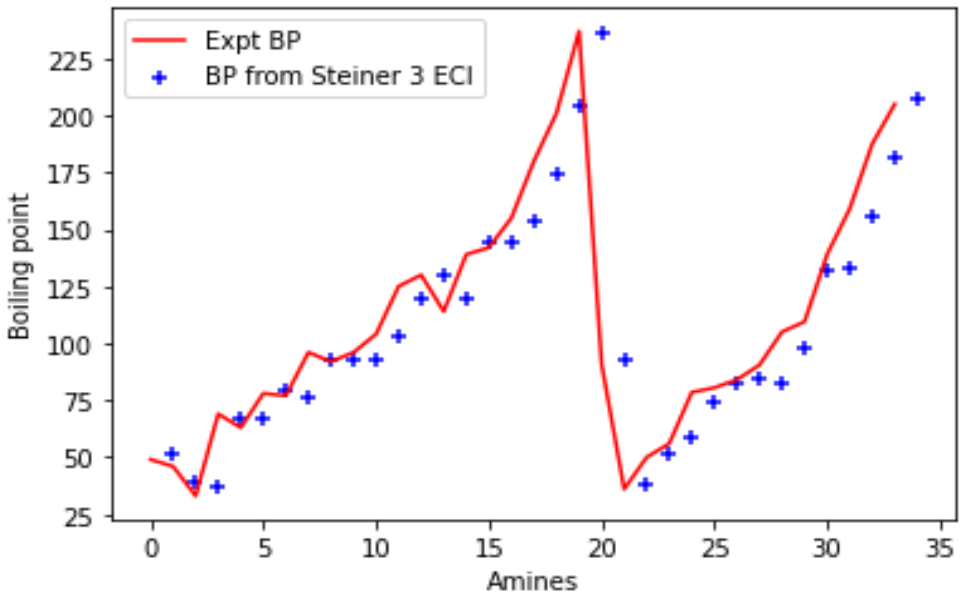

Figure 1: Comparison plot for BP of amines using Steiner 3-eccentric connectivity index and eccentric connectivity index.

Table 5: Comparison for cross section area of alcohols using Steiner 3-eccentric connectivity index and eccentric connectivity index.

				Predicted CSA	
Compound	ξ_3^c	ξ^c	expt	ξ_3^c	ξ^c
2-methyl propanol	27	19	263.8	264.53	264.29
2-butanol	27	19	264.1	264.53	264.29
2-pentanol	41	31	295.9	295.71	299.52
2-methyl 2-butanol	34	24	282.5	281.35	280.62
1-hexanol	72	54	335.7	338.75	340.14
2-methyl 2-pentanol	52	38	314.3	314.15	314.66
2-methyl 3-pentanol	51	36	314.3	312.65	310.67
4-methyl 2-pentanol	52	38	314.9	314.15	314.66
1-heptanol	98	74	367.5	365.13	368.20
2,3-dimethyl 2-pentanol	61	43	323.8	326.31	323.69
3-heptanol	87	63	357.1	353.76	352.16
2,6-dimethyl 4-heptanol	113	83	394.0	383.88	384.80
2-ethyl hexanol	108	77	371.3	377.03	373.27
3,5,5-trimethyl hexanol	113	83	376.6	383.87	384.80

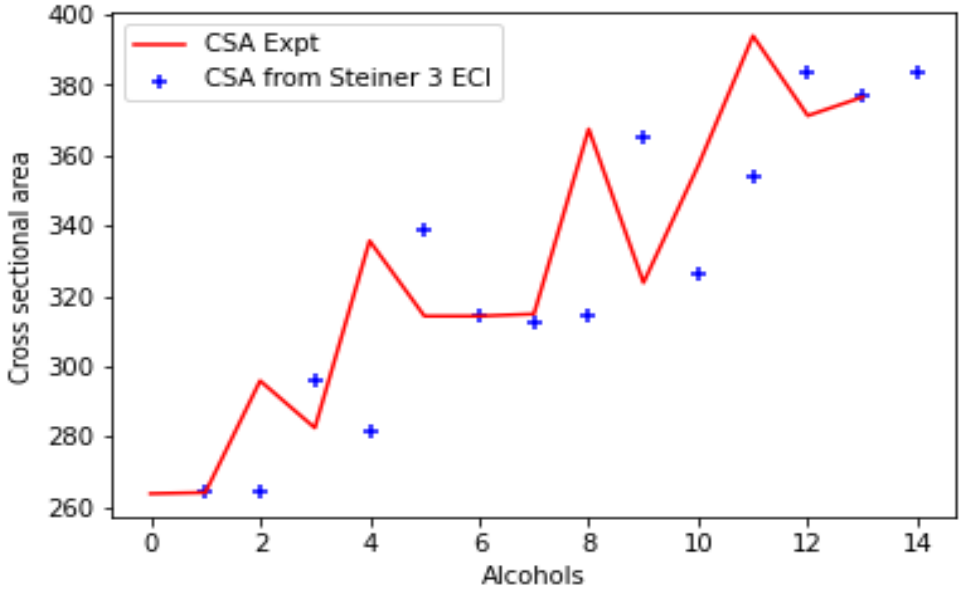

Figure 2: Comparison plot for Cross sectional area of alcohols using Steiner 3-eccentric connectivity index and eccentric connectivity index.

Table 6: Regression statistics for Cross sectional area (CSA) of alcohols.

Properties	CSA of alcohols from ξ_3^c
Multiple R	0.99505
R^2	0.99013
Adjusted R^2	0.98834
CC(%)	99.50547
Avg error (%)	0.78752
RMS error(%)	1.07038
F	100.35839

The regression equation for Cross sectional area of alcohols is

$$CSA = 1.702 \times 10^2 + 4.519\xi_3 - 4.25 \times 10^{-2}\xi_3^2 + 1.704 \times 10^{-4}\xi_3^3. \quad (4)$$

Table 7: Comparison for molar refraction of alcohols using Steiner 3-eccentric connectivity index and eccentric connectivity index.

				Predicted MR	
Compound	ξ_3^c	ξ^c	expt	ξ_3^c	ξ^c
3-methyl 1-butanol	41	31	26.90	28.04	28.49
2-methyl 2-butanol	34	24	26.72	26.19	27.58
2-methyl 1-pentanol	63	45	31.16	32.94	32.48
2,2-dimethyl 1-butanol	52	34	31.27	30.64	29.14
3-methyl 3-pentanol	52	34	31.18	30.64	29.14
2-methyl 1-hexanol	87	63	35.93	37.38	38.85
3-ethyl 3-pentanol	69	54	35.82	34.10	35.74
4-ethyl 4-heptanol	121	77	44.92	43.88	42.02
6-methyl 1-heptanol	115	87	40.74	42.61	41.98
3-methyl 3-heptanol	99	66	40.45	39.53	39.76
4-methyl 4-heptanol	99	68	40.44	39.53	40.30

Table 8: Regression statistics for molar refraction of alcohols.

Properties	MR of alcohols from ξ_3^c
Multiple R	0.97709
R^2	0.95472
Adjusted R^2	0.94339
CC(%)	97.70957
Avg error (%)	3.26285
RMS error(%)	3.53606
F	21.0829

The regression equation for molar refraction of alcohols is

$$MR = 14.18 + 0.443\xi_3 - 3.047 \times 10^{-3}\xi_3^2 + 1.166 \times 10^{-5}\xi_3^3. \quad (5)$$

From Tables 1 to 8 we can observe that the Steiner 3-eccentric connectivity index has a very good correlating ability due to its minimal average and RMS errors. We conclude that Steiner 3-eccentric connectivity index has better predicting ability in finding boiling points of both primary and secondary amines, cross-sectional area and molar refraction of some alcohols than the eccentric connectivity index. Comparison plots are given in Figures 1 to 3.

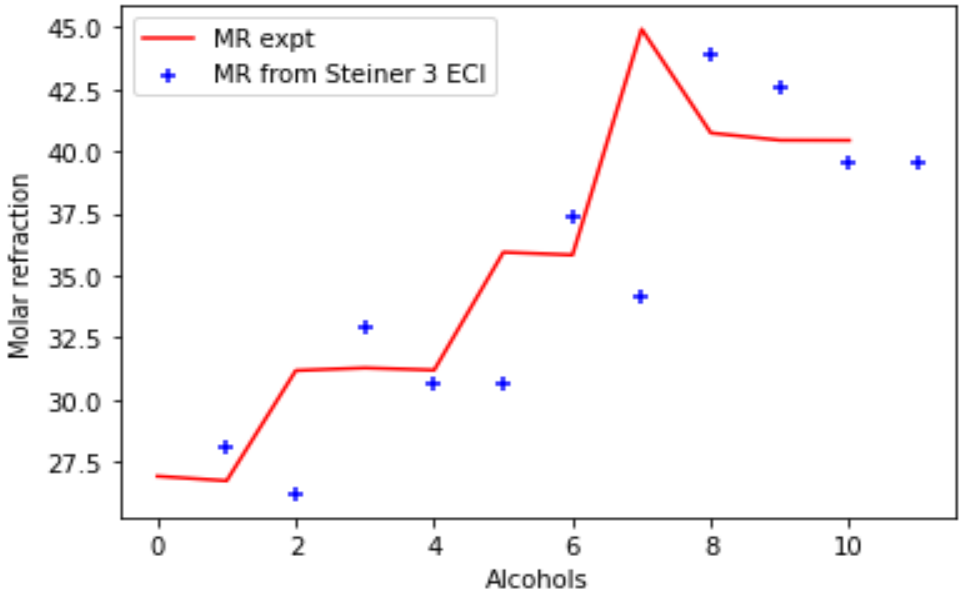

Figure 3: Comparison plot for Molar refraction of alcohols using Steiner 3-eccentric connectivity index and eccentric connectivity index.

5 Conclusion

In this paper, we have introduced a novel, generalized distance-based invariant named Steiner k-eccentric connectivity index and we have derived closed-form values of many standard classes of graphs. On the application front of the newly defined index, we have proved that the Steiner 3-eccentric connectivity index is a better predictor for finding the boiling points of considered primary and secondary amines, cross sectional area of alcohols, molar refraction of alcohols with correlation coefficient more than 97% for each. In the future, these analyses can be extended for higher-order Steiner k-eccentric connectivity index to get a better prediction of the physico chemical properties of different chemicals.

Conflicts of interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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