Research Article

Hani Shaker, Muhammad Imran*, and Wasim Sajjad

Eccentricity based topological indices of face centered cubic lattice $FCC(n)$

https://doi.org/10.1515/mgmc-2021-0005
received February 18, 2020; accepted November 26, 2020

Abstract: Chemical graph theory has become a prime gadget for mathematical chemistry due to its wide range of graph theoretical applications for solving molecular problems. A numerical quantity is named as topological index which explains the topological characteristics of a chemical graph. Recently face centered cubic lattice $FCC(n)$ attracted large attention due to its prominent and distinguished properties. Mujahed and Nagy (2016, 2018) calculated the precise expression for Wiener index and hyper-Wiener index on rows of unit cells of $FCC(n)$. In this paper, we present the $ECI$ (eccentric-connectivity index), $TCI$ (total-eccentricity index), $CEI$ (connective eccentric index), and first eccentric Zagreb index of face centered cubic lattice.

Keywords: eccentric-connectivity index, total-eccentricity index, connective eccentric index, first eccentric Zagreb index, $FCC(n)$

1 Introduction

Mathematical chemistry has an important branch called chemical graph theory. The significantly large applications of graph theory can solve molecular questions that are related to the support of the chemical graph theory. Its founders are Ante Graovac et al. (1977), Alexandru Balaban (1982), Haruo Hosoya (1971), Milan Randić (1975), Ivan Gutman, and Nenad Trinajstić (Gutman and Trinajstić, 1972). A chemical system is a model which

denotes a chemical graph which explains the relationship between its components such as atoms, bonds, group of atoms, or molecules. In a chemical graph we represent atoms as graph vertices and atom bonds as graph edges. Algebraic invariants in chemical graph theory are used to describe the structural properties of a molecule that describes the molecule strength, structural fragments, molecular branching, and electronic configurations. These theoretical graph invariants are associated with the physical analysis determined by experimentation (Bonchev, 1991). Such mathematical and computing ways are used at the atomic level to evaluate and develop a matter’s structure. Chemical graph theory provides a large number of complementary and necessary tools for the better understanding of chemical structures and emerged as a useful contributor to the theoretical chemistry.

A $G = (V, E)$ graph is a collection of $V$ points called a vertex set, and a selection of two $V$ points subsets called an edge set. A strict graph, i.e. undirected connected with no multi edges and with no loops, having $n = |V|$ vertices and $m = |E|$ edges is known as a molecular graph. The atoms are identified by $v \in V$, with $(v, v) \in E$ representing the covalent bonds between the corresponding atoms. The hydrocarbons also contain carbon and hydrogen atoms with their molecular graphs reflect the carbon structure of the molecule (Balaban, 2013; Bonchev, 1991). In a graph $G$, a walk is an alternative sequence of graph vertices starting from the vertex $u$ and ending at the vertex $v$, sometimes called the $u$–$v$ walk. A $u$–$v$ path is a walk if there are no vertices repeated. In a path, the number of edges is termed as the length of the path. The idea of path length in a graph leads us to define the distance between two vertices. The total number of edges in a shortest $u$–$v$ path in a graph $G$ is called the distance from vertex $u$ to vertex $v$, which is denoted by $d(u, v)$ where $u, v \in G$. Vertex $u$’s eccentricity $\varepsilon(u)$ is the distance between $u$ and a vertex that is farthest from $u$ in the connected graph $G$.

One can characterize a graph by a numerical number, sequence of numbers, polynomial, or matrix. A numerical quantity correlated with a graph describing network topology and being invariant within graph automorphism
Eccentricity based topological indices of face centered cubic lattice $FCC(n)$

is called a topological index. One may think of the topological index associated to a graph $G$ as of a number with the characteristic that for every graph $H$ isomorphic to $G$, “$\text{Top}(H) = \text{Top}(G)$” is a topological index $\text{Top}(G)$ of a graph (Deza, 2000). Some popular categories of topological indices include topological indices based on distance/ eccentricity and topological indices based on degree.

This theory of indices began with the Wiener index, the first index proposed by Wiener (1947) who worked with the boiling point of a material namely paraffin. This index was completely dependent on the distance between the vertices of the chemical graph so he labeled it path number but afterwards it was renamed as $W$ denoted Wiener index. Wiener stated that a path number is called the sum of the distances between all pairs of atoms. Algebraically, the Wiener index for a graph $G$ is:

$$W(G) = \sum_{(u,v) \in G} d(u,v)$$

Eccentricity based topological indices have high importance in the chemical graph theory. Sharma et al. (1997) proposed a significant eccentricity based topological index, called eccentric-connectivity index $\xi(G)$ and defined as:

$$\xi(G) = \sum_{u \in V(G)} d(u)e(u)$$

where: $d(u)$ represents the degree of the vertex $u$ and $e(u)$ represents the eccentricity of the vertex $u$ in graph $G$. Ashrafi and Saheli (2010) and Saheli and Ashrafi (2010) computed the eccentric connectivity index of a new class of dendrimers and Armchair Polyhex. De (2012) computed the eccentric connectivity index of thorn graph. Nadeem and Shaker (2016) computed the eccentric connectivity index of TiO$_2$ nanotube. The total-eccentricity index of a graph $G$ is defined when we do not consider the vertex degree. The total-eccentricity index for a graph $G$ is:

$$\tau(G) = \sum_{u \in V(G)} e(u)$$

Zobair et al. (2018) computed the total connectivity index of triangulane dendrimers. Connective eccentric index is another significant eccentricity based index denoted by $C^e(G)$ which was described in Gupta et al. (2000, 2002a, 200b). The connective eccentric index is defined as:

$$C^e(G) = \sum_{u \in V(G)} d(u)/e(u)$$

Huo et al. (2017) computed connective eccentric index of $NAm$ nanotube. NAm$^n$ nanotube has been discussed by Dhavaseelan et al. (2017) and Farahani et al. (2018). Farahani (2014) computed connective eccentric index of an infinite family of linear polyene parallelogram benzenoid. The first eccentric Zagreb index of a molecular graph $G$ was introduced in Ghorbani and HosseinZadeh (2012). The first eccentric Zagreb index is described in terms of eccentricity:

$$M_1(G) = \sum_{u \in V(G)} [e(u)]^2$$

Kulandai (2015) computed first and second Zagreb indices of corona graph. Foruzanfar et al. (2017) computed first eccentric Zagreb index of the $N^m{[\mathcal{D}]}$ growth of the nanostar dendrimer $D_{[\mathcal{D}]}$. In this paper we consider the chemical graph of face centered cubic lattice $FCC(n)$ and calculate some important eccentricity based topological indices such as $ECI$ (eccentric-connectivity index), $TCI$ (total-eccentricity index), $CEI$ (connective eccentric index), and first eccentric Zagreb index.

2 Face centered cubic lattice $FCC(n)$

Face centered cubic (FFC) lattice is formed by unit cells that are cubes with an atom at each corner of the cube and an atom in the centre of each face of the cube. Each center atom of the cube has bounds with the closest atoms. The graph of $FCC$ is presented in Figure 1 where vertices represent the atoms and edges indicate the bounds between the atoms. As a structure, FCC has the largest

Figure 1: $FCC(1)$: A unit cell of face-centered cubic (FCC) lattice.
packing density in 3D space. Because of its largest packing density, FCC is one of the most well-organized structures to pack same size of spheres in a volume. FCC structure is also known as cubic closest-packed crystal structure. Metals with FCC structure include: aluminum, copper, gold, nickel, and silver.

Figure 2 represents a row of \( n \) unit cells of the FCC lattice, we denote it as FCC\((n)\). FF(1) represents a face centered cubic. The molecular graph of FCC\( (n) \) consists of total \( 9n+5 \) vertices and \( 32n+4 \) edges between the vertices. In recently published articles on FCC\( (n) \), Mujahed and Nagy (2016, 2018) calculated the precise expression for Wiener index and hyper-Wiener index on rows of unit cells of face centered cubic lattice. We consider the eccentricities of the molecular graph of FCC\( (n) \) and compute some important eccentricity based topological indices for FCC\( (n) \).

Throughout this paper we use the following representation for the vertices of the molecular graph of FCC\( (n) \):

\[
V = \{v'_i | 1 \leq i \leq n+5 \} \cup \{u'_j | 1 \leq j \leq n, 1 \leq i \leq 4 \}
\]

where \( v'_i \) represents the vertices on the left and right sides of each cube of FCC\( (n) \) and \( u'_j \) represents the center vertices of rest of the sides of each cube of FCC\( (n) \). For better understanding see Figures 1 and 2.

3 Main results

In this section we present our main results in which we provide the complete computation of the eccentric-connectivity index, total-eccentricity index, connective eccentric index, and first eccentric Zagreb index of FCC\( (n) \). We make partitions of the graph of FCC\( (n) \) according to even and odd values of \( n \) and then calculate the eccentricity based topological indices of graph. We arrange our calculation tables according to

\( n \equiv 0(\text{mod}2) \) and \( n \equiv 1(\text{mod}2) \). For every index we have two calculation tables: one for \( n \equiv 0(\text{mod}2) \) and other for \( n \equiv 1(\text{mod}2) \).

3.1 Eccentric-connectivity index of FCC\( (n) \)

Theorem 1
For any graph \( G \cong \text{FCC}(n) \), where \( n \equiv 0(\text{mod}2) \). Then:

\[
\xi(G) = 112n + 128 \sum_{j=0}^{n-1} (j+1) + 64 \sum_{j=0}^{n-1} (2j+1)
\]

Proof: Consider the graph of FCC\( (n) \) where \( n \equiv 0(\text{mod}2) \) and labeled it as \( G \). Using the values from Table 1 in the expression of ECI stated in Eq. 2, we obtain:

\[
\xi(G) = (8 \times 3 \times 2n) + (2 \times 8 \times 2(n-1)+2)
\]

After simplification, we get:

\[
\xi(G) = 112n + 128 \sum_{j=0}^{n-1} (j+1) + 64 \sum_{j=0}^{n-1} (2j+1)
\]

Theorem 2
For any graph \( G \cong \text{FCC}(n) \), where \( n \equiv 1(\text{mod}2) \). Then:

\[
\xi(G) = 80n + 48 \sum_{j=0}^{n-1} (j+1) + 80 \sum_{j=0}^{n-1} (j+1) + 64 \sum_{j=0}^{n-1} (2j+1)
\]

Proof: Consider the graph of FCC\( (n) \) where \( n \equiv 0(\text{mod}2) \) and labeled it as \( G \). Using the values from Table 1 in the expression of ECI stated in Eq. 2, we obtain:
Eccentricity based topological indices of face centered cubic lattice

**Proof:** Consider the graph of $FCC(n)$ where $n \equiv 1 \pmod{2}$ and labeled it as $G$. Using the values from Table 2 in the expression of ECI stated in Eq. 2, we obtain:

$$\zeta(G) = (8\times3\times2n) + 2\times8\times\sum_{j=n-1}^{n-2} (2j+2) + 2\times12\times\sum_{j=n-1}^{n-2} (2j+2)$$

$$+ 8\times5\times\sum_{j=n-1}^{n-2} (2j+2) + 8\times8\times\sum_{j=n-1}^{n-2} (2j+1)$$

After simplification, we get:

$$\zeta(G) = 80n + 48\sum_{j=n-1}^{n-2} (j+1) + 80\sum_{j=n-1}^{n-2} (j+1) + 64\sum_{j=n-1}^{n-2} (2j+1)$$

### 3.2 Total-eccentricity index of $FCC(n)$

**Theorem 3**

For any graph $G \equiv FCC(n)$, where $n \equiv 0 \pmod{2}$. Then:

$$\zeta(G) = 5n + \sum_{j=0}^{n} (36j + 28)$$

**Proof:** Consider the graph of $FCC(n)$ where $n \equiv 0 \pmod{2}$ and labeled it as $G$. Using the values from Table 3 in the expression of TEC stated in Eq. 3, we obtain:

$$\zeta(G) = 10\times\sum_{j=0}^{n} (2j+2) + 8\times\sum_{j=0}^{n} (2j+1) + (4\times n) + (1\times n)$$

After simplification, we get:

$$\zeta(G) = 5n + \sum_{j=0}^{n} (36j + 28)$$

### Table 1: Eccentricity and degree based vertex partition of $FCC(n)$ for $n \equiv 0 \pmod{2}$

| Representatives | Degree | Eccentricity | Range | Frequency |
|----------------|--------|--------------|--------|-----------|
| $\{v^{n-1}_i, v^{i+2}_j\}$ | 3      | $2n$         | $j = n - 1, 1 \leq i \leq 4$ | 8         |
| $\{v^{n-1}_i, v^{i+2}_j\}$ | 8      | $2j + 2$     | $\frac{n-1}{2} \leq j \leq n - 1$ | 2 for each $j$ |
| $\{v^{n-1}_i, v^{i+2}_j\}$ | 12     | $2j + 2$     | $\frac{n-1}{2} \leq j \leq n - 1, 1 \leq i \leq 4$ | 8 for each $j$ |
| $\{v^{i}_j\}$ | 5      | $n$          | $j = \frac{n}{2} + 1, 1 \leq i \leq 4$ | 4         |
| $\{v^{i}_j\}$ | 12     | $n$          | $j = \frac{n}{2} + 1$ | 1         |

### Table 2: Eccentricity and degree based vertex partition of $FCC(n)$ for $n \equiv 1 \pmod{2}$

| Representatives | Degree | Eccentricity | Range | Frequency |
|----------------|--------|--------------|--------|-----------|
| $\{v^{n-1}_i, v^{i+2}_j\}$ | 3      | $2n$         | $j = n - 1, 1 \leq i \leq 4$ | 8         |
| $\{v^{n-1}_i, v^{i+2}_j\}$ | 8      | $2j + 2$     | $\frac{n-1}{2} \leq j \leq n - 1$ | 2 for each $j$ |
| $\{v^{n-1}_i, v^{i+2}_j\}$ | 12     | $2j + 2$     | $\frac{n-1}{2} \leq j \leq n - 1, 1 \leq i \leq 4$ | 2 for each $j$ |
| $\{v^{n-1}_i, v^{i+2}_j\}$ | 5      | $2j + 2$     | $\frac{n-1}{2} \leq j \leq n - 1, 1 \leq i \leq 4$ | 8 for each $j$ |
| $\{v^{n-1}_i, v^{i+1}_j\}$ | 8      | $2j + 1$     | $\frac{n-1}{2} \leq j \leq n - 1, 1 \leq i \leq 4$ | 8 for each $j$ |

### Table 3: Eccentricity based vertex partition of $FCC(n)$ for $n \equiv 0 \pmod{2}$

| Representatives | Eccentricity | Range | Frequency |
|----------------|--------------|--------|-----------|
| $\{v^{n-1}_i, v^{i+2}_j\}$ | $2j + 2$ | $\frac{n-1}{2} \leq j \leq n - 1, 1 \leq i \leq 5$ | 10 for each $j$ |
| $\{v^{n-1}_i, v^{i+1}_j\}$ | $2j + 1$ | $\frac{n-1}{2} \leq j \leq n - 1, 1 \leq i \leq 4$ | 8 for each $j$ |
| $\{v^{i}_j\}$ | $3$          | $j = \frac{n}{2} + 1, 1 \leq i \leq 4$ | 4 for each $j$ |
| $\{v^{i}_j\}$ | $n$          | $j = \frac{n}{2} + 1$ | 1         |
Table 4: Eccentricity based vertex partition of FCC(n) for \( n \equiv 1 \pmod{2} \)

| Representatives | Eccentricity | Range | Frequency |
|-----------------|-------------|-------|-----------|
| \((v^1_i, v^2_j)\) | 2\(j+2\) | \(\frac{n+1}{2} \leq j \leq n-1\), 1\(\leq i \leq 5\) | 10 for each \(j\) |
| \((u^1_j, u^2_i)\) | 2\(j+1\) | \(\frac{n+1}{2} \leq j \leq n-1\), 1\(\leq i \leq 4\) | 8 for each \(j\) |
| \((u^1_i)\) | \(n\) | \(j = \frac{n+1}{2}\), 1\(\leq i \leq 4\) | 4 |

Theorem 4

For any graph \( G \cong \text{FCC}(n) \), where \( n \equiv 1 \pmod{2} \).

\[
\zeta(G) = 4n + 20 \sum_{j=\frac{n-1}{2}}^{\frac{n+1}{2}} (j+1) + 8 \sum_{j=\frac{n+1}{2}}^{\frac{n-1}{2}} (2j+1)
\]

Proof: Consider the graph of \( \text{FCC}(n) \) where \( n \equiv 1 \pmod{2} \) and labeled it as \( G \). Using the values from Table 4 in the expression of TEC stated in equation 3, we obtain:

\[
\zeta(G) = 10 \sum_{j=\frac{n-1}{2}}^{\frac{n+1}{2}} (2j+2) + 8 \sum_{j=\frac{n+1}{2}}^{\frac{n-1}{2}} (2j+1) + (4 \times n)
\]

After simplification, we get:

\[
\zeta(G) = 4n + 20 \sum_{j=\frac{n-1}{2}}^{\frac{n+1}{2}} (j+1) + 8 \sum_{j=\frac{n+1}{2}}^{\frac{n-1}{2}} (2j+1)
\]

3.3 Results for connective eccentric index of \( \text{FCC}(n) \)

Theorem 5

For any graph \( G \cong \text{FCC}(n) \), where \( n \equiv 0 \pmod{2} \).

\[
C^5(G) = \frac{52}{n} \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} \frac{32}{j+1} + \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} \frac{64}{2j+1}
\]

Proof: Consider the graph of \( \text{FCC}(n) \) where \( n \equiv 0 \pmod{2} \) and labeled it as \( G \). Using the values from Table 3 in the expression of CEI stated in Eq. 4, we obtain:

\[
C^5(G) = 8 \times \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} \frac{3}{2n} + 2 \times \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} \frac{8}{2j+2} + 8 \times \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} \frac{5}{2j+2}
\]

After simplification, we get:

\[
C^5(G) = \frac{20}{n} \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} \frac{12}{j+1} + \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} \frac{20}{j+1} + \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} \frac{64}{2j+1}
\]

3.4 Results for first eccentric Zagreb index of \( \text{FCC}(n) \)

Theorem 6

For any graph \( G \cong \text{FCC}(n) \), where \( n \equiv 1 \pmod{2} \).

\[
M_1'(G) = 5n^3 + \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} (72j^2 + 112j + 48)
\]

Proof: Consider the graph of \( \text{FCC}(n) \) where \( n \equiv 0 \pmod{2} \) and labeled it as \( G \). Using the values from Table 3 in the expression of first eccentric Zagreb index stated in Eq. 5, we obtain:

\[
M_1'(G) = 10 \times \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} (2j+2)^3 + 8 \times \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} (2j+1)^3
\]

After simplification, we get:

\[
M_1'(G) = \left[ 10 \times \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} (2j+2)^3 \right] + \left[ 8 \times \sum_{j=\frac{n}{2}}^{\frac{n+1}{2}} (2j+1)^3 \right] + \left[ 4 \times n^3 \right] + \left[ 1 \times n^3 \right]
\]
After simplification, we get:

\[ M_1(G) = 5n^2 + \sum_{j=2}^{n-1} (72j^2 + 112j + 48) \]

**Theorem 8**

For any graph \( G \equiv FCC(n) \), where \( n \equiv 1(\text{mod}2) \). Then:

\[ M_1(G) = 4n^2 + \sum_{j=2}^{n-1} (40j^2 + 80j + 40) + \sum_{j=2}^{n-1} (32j^2 + 32j + 8) \]

**Proof:** Consider the graph of \( FCC(n) \) where \( n \equiv 1(\text{mod}2) \) and labeled it as \( G \). Using the values from Table 4 in the expression of first eccentric Zagreb index stated in Eq. 5, we obtain:

\[
M_1(G) = \left[ 10 \times \sum_{j=2}^{n-1} (2j+2)^2 \right] + \left[ 8 \times \sum_{j=2}^{n-1} (2j+1)^2 \right] + [4 \times n^2]
\]

After simplification, we get:

\[ M_1(G) = 4n^2 + \sum_{j=2}^{n-1} (40j^2 + 80j + 40) + \sum_{j=2}^{n-1} (32j^2 + 32j + 8) \]

4 Conclusion

In QSPR/QSAR studies, eccentricity-based topological indices are very useful and effective, particularly the eccentric connectivity index offers excellent accuracy compared to other indices in numerous biological activities. In this paper, the eccentric-connectivity index, the total-eccentricity index, the connective eccentric index, and the first eccentricity-based Zagreb index were analyzed and computed for the \( FCC(n) \) graph of face-centered cubic lattice.

**Acknowledgment:** The authors are very grateful to the referees for their constructive suggestions and useful comments, which improved this work very much.

**Research funding:** This research is supported by Higher Education Commission Pakistan via Grant No. 5331/Federal/NRPU/R and D/HEC/2016, and UPAR Grant of UAEU, UAE via Grant No. G00003271.

**Author contribution:** Hani Shaker: writing – original draft, writing – review and editing, methodology, computational analysis; Muhammad Imran: writing – original draft, formal analysis, visualization, project administration; Wasim Sajjad: writing – original draft, writing and editing, computations and formulation.

**Conflict of interest:** One of the authors (Muhammad Imran) is a Guest Editor of the Main Group Metal Chemistry’s Special Issue “Topological descriptors of chemical networks: Theoretical studies” in which this article is published.

**Data availability statement:** All the data is available in this manuscript.

**References**

Ashrafi A.R., Saheli M., The eccentric connectivity index of a new class of nanostar dendrimers. Optoelectron. Adv. Mater Rapid Comm., 2010, 4(6), 898-899.

Bonchev D., Chemical graph theory. Gordon and Breach Publishers S.A., 1991.

Balaban A.T., Chemical graph theory and sherlock holmes principle. HYLE, 2013, 19, 107-134.

Balaban A.T., Distance connectivity index. Chem. Phys. Lett., 1982, 89, 399-404.

Deza M., Fowler P.W., Rassat A., Rogers K.M., Fullerenes as tiling of surfaces. J. Chem. Inf. Comput. Sci., 2000, 40, 550-558.

De N., On eccentric connectivity index and Polynomial of Thorn Graph. Appl. Math., 2012, 3, 931-934.

Dhavaseelan R., Baig A.Q., Sajjad W., Farahani M.R., Eccentric connectivity polynomial and Total eccentricity polynomial of \( \text{N}^n \text{A}_m \) nanotube. J. Inf. Math. Sci., 2017, 9(1), 201-215.

Farahani M.R., Connective eccentric index of an infinite family of linear polyene parallelogram benzenoid. Int. Lett. Chem.-Phys. Aastr., 2014, 18, 57-62.

Farahani M.R., Baig A.Q., Sajjad W., Ramane H.S., Eccentricity version of atom-bond connectivity index of \( \text{N}^n \text{A}_m \) nanotube. Int. J. Adv. Math., 2018, 2018(1), 101-108.

Foruzanfar Z., Farahani M.R., Baig A.Q., Sajjad W., The first eccentric Zagreb index of the \( \text{N}^n \) growth of the nanostar dendrimer \( D_{[D]} \). Int. J. Pure Appl. Math., 2017, 117(1), 99-106.

Graovac A., Gutman I., Trinajstic N., Topological Approach to the Chemistry of Conjugated Molecules, In: Lecture Notes in Chemistry (Vol. 4). Springer-Verlag, Berlin, 1977.

Gupta S., Singh M., Madan A.K., Application of graph theory: Relationship of eccentric connectivity index and Wiener’s index
with anti-inflammatory activity. J. Math. Anal. Appl., 2002a, 266, 259-268.
Gupta S., Singh M., Madan A.K., Connective eccentricity index: a novel topological descriptor for predicting biological activity. J. Mol. Graph. Model., 2000, 18, 18-25.
Gupta S., Singh M., Madan A.K., Application of Graph Theory: Relationship of Eccentric Connectivity Index and Wiener’s Index with Anti-inflammatory Activity. J. Math. Anal. Appl., 2002b, 266, 259-268.
Gutman I., Trinajstic N., Graph theory and molecular orbitals and Total π-electron energy of alternant hydrocarbons. Chem. Phys. Lett., 1972, 17, 535-538.
Ghorbani M., Hosseinzadeh M.A., A new version of Zagreb indices. Filomat, 2012, 26(1), 93-100.
Hosoya H., Topological index, Bull. Chem. Soc. Japan, 1971, 44, 2332-2339.
Huo Y., Liu J.B., Baig A.Q., Sajjad W., Farahani M.R., Connective Eccentric Index of \( N_{Am} \) Nanotube. J. Comput. Theor. Nanos., 2017, 14, 1832-1836.
Kulandai A., Eccentric connectivity index, First and second Zagreb indices of Corona Graph. Int. J. Math. Comput. Phys. Elec. Comp. Eng., 2015, 9(1), 71-75
Mujahed H., Nagy B., Wiener index on rows of unit cells of the face-centred cubic lattice. Acta Crystallogr. A, 2016, A72(2), 243-249.
Mujahed H., Nagy B., Exact formula for computing the Hyper-Wiener index on Rows of unit cells of the face-centred cubic lattice. An. St. Univ. Ovidius Constanta-Seria Matematica, 2018, 26(1), 169-187.
Nadeem I., Shaker H., On eccentric connectivity index of TiO\(_2\) nanotubes. Acta Chim. Slov., 2016, 63, 363-368.
Randić M., On Characterization of molecular branching. J. Amer. Chem. Soc., 1975, 97, 6609-6615.
Saheli M., Ashrafi A.R., The eccentric connectivity index of Armchair Polyhex Nanotubes. Maced. J. Chem. Chem. En., 2010, 29(1), 71-75.
Sharma V., Goswami R., Madan A.K., Eccentric connectivity index: A novel highly discriminating topological descriptor for structure-property and structure-activity studies. J. Chem. Inf. Comput. Sci., 1997, 37, 272-282.
Wiener H., Structural determination of paraffin boiling points. J. Amer. Chem. Soc., 1947, 69, 17-20.
Zobair M.M., Ali M.M., Shaker H., Rehman, N., Eccentricity based topological invariants of triangulane dendrimers. Utilitas Mathematica, 2018, 107, 193-206.