Eccentric Distance Sum in Chemical Compounds Graph Using Domination

Chapter · May 2021

DOI: 10.1007/978-981-33-4389-4_3

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M. Raji and G. Jayalalitha

Abstract Any graphical representation of combined points and connecting lines is called a graph. Railway networks, mobile communication networks and any other traffic connections are more often examples. The representation of an atomic structure by a graph, which is connected, undirected and their vertices represent atoms and their edges are bondings, is an important application of graph theory field called chemical graph theory. Chemical graph theory is often used through the interpretation of chemical structures into numerical graph invariants. Graph invariant is a property of the graph that is preserved by isomorphism. Eccentric distance sum is a novel graph invariant which can be used in chemical compounds structure, some drug designs and molecular documentation. Eccentric distance sum presents a huge potential for structure relationships. This paper shows eccentric distance sum in the graph of chemical compounds that depends on minimum dominating distance matrix and then computes total eccentricity of linear benzenoid system (LBS) for h hexagons where $h \leq 5$.

Keywords Distance in graphs · Minimum dominating distance matrix · Eccentric distance sum

1 Introduction

Let G be molecular graph where atoms and bonds are specified by vertices and edges, respectively [1]. Graph theory may be employed through the translation of chemical structures into characteristic polynomial, matrix, sequence and numerical graph invariants [2–5]. Gupta, Singh and Madan established eccentric distance sum [6]. Throughout this paper, graphs are taken into consideration as simple, connected,

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S.-L. Peng et al. (eds.), *Proceedings of First International Conference on Mathematical Modeling and Computational Science*, Advances in Intelligent Systems and Computing 1292, https://doi.org/10.1007/978-981-33-4389-4_3

finite and undirected graphs. Graph theory is one among the foremost developing branches of recent mathematics and computer applications. The theory of domination has been an important part of research activity in graph theory. Domination in graphs has applications to many fields like engineering, basic sciences, life sciences, etc. For a graph G and a subset D of the vertex set $V(G)$, the set of vertices in G is in D or adjacent to a vertex in D. Then D is called a dominating set. The details about dominating set and minimum dominating distance matrix of G can be found in [7–10]. The eccentricity of a vertex v, $e(v)$ is the maximum distance from v to any other vertex [11]. Total eccentricity of the graph G, TE (G), is defined as the summation of eccentricities of all vertices of graph G [12]. Eccentric distance sum EDS (G) can be stated as the total number of the product of eccentricity and distance sum of each vertex in a graph G [6].

2 Eccentric Distance Sum in Graph of Chemical Compounds

Here it describes the computation of eccentric distance sum in the graph of chemical compounds like benzene, naphthalene and anthracene using minimum dominating distance matrix.

2.1 Molecular Graph of Benzene

The structure of benzene consists of six vertices. Its vertices are of degree 2. So all vertices have even degree. The maximum distance of each vertex to another vertex is 3 (Fig. 1 and Table 1).

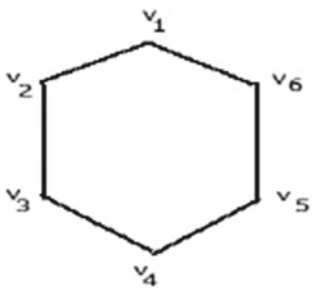

Fig. 1 Benzene

Table 1 Eccentricity of molecular graph of benzene

$e(v_i)$ $(i = 1–6)$	3	3	3	3	3	3

TE (Benzene) = 3 + 3 + 3 + 3 + 3 + 3 = 18.
EDS (Benzene) = 27 + 27 + 30 + 27 + 27 + 30 = 168.

Minimum Dominating Distance Matrix (6 × 6) of Benzene

$$\begin{pmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 1 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 1 \end{pmatrix}$$

2.2 Molecular Graph of Naphthalene

The structure of naphthalene consists of ten vertices. Its vertices have degree 2 and 3. In this, eight vertices are of degree 2 and two vertices are of degree 3 (Fig. 2 and Table 2).

Minimum Dominating Distance Matrix (10 × 10) of Naphthalene

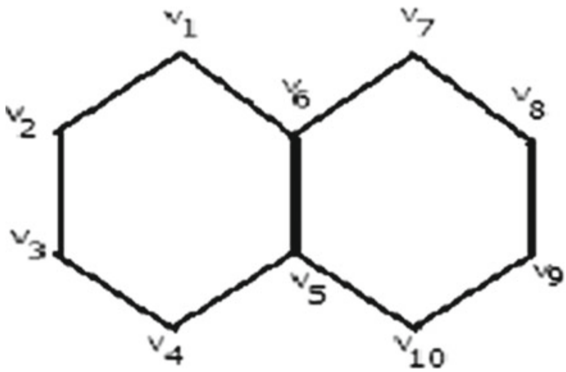

Fig. 2 Naphthalene

Table 2 Eccentricity of molecular graph of naphthalene

$e(v_1)$	$e(v_2)$	$e(v_3)$	$e(v_4)$	$e(v_5)$	$e(v_6)$	$e(v_7)$	$e(v_8)$	$e(v_9)$	$e(v_{10})$
4	5	5	4	3	3	4	5	5	4

TE (Naphthalene) = 4 + 5 + 5 + 4 + 3 + 3 + 4 + 5 + 5 + 4 = 42
EDS (Naphthalene) = 84 + 125 + 130 + 84 + 51 + 54 + 84 + 125 + 130 + 84 = 951

$$\begin{pmatrix} 0&1&2&3&2&1&2&3&4&3\\ 1&0&1&2&3&2&3&4&5&4\\ 2&1&1&1&2&3&4&5&4&3\\ 3&2&1&0&1&2&3&4&3&2\\ 2&3&2&1&0&1&2&3&2&1\\ 1&2&3&2&1&1&1&2&3&2\\ 2&3&4&3&2&1&0&1&2&3\\ 3&4&5&4&3&2&1&0&1&2\\ 4&5&4&3&2&3&2&1&1&1\\ 3&4&3&2&1&2&3&2&1&0 \end{pmatrix}$$

2.3 Molecular Graph of Anthracene

The structure of anthracene consists of 14 vertices. Its vertices have degree 2 and 3. Here, ten vertices are of degree 2 and four vertices are of degree 3 (Fig. 3 and Table 3).

Minimum Dominating Distance Matrix (14 × 14) of Anthracene

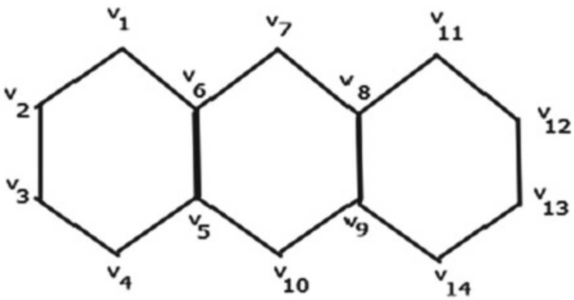

Fig. 3 Anthracene

Table 3 Eccentricity of molecular graph of Anthracene

$e(v_1)$	$e(v_2)$	$e(v_3)$	$e(v_4)$	$e(v_5)$	$e(v_6)$	$e(v_7)$	$e(v_8)$	$e(v_9)$	$e(v_{10})$	$e(v_{11})$	$e(v_{12})$	$e(v_{13})$	$e(v_{14})$
6	7	7	6	5	5	4	5	5	4	6	7	7	6

TE (Anthracene) $= 6 + 7 + 7 + 6 + 5 + 5 + 4 + 5 + 5 + 4 + 6 + 7 + 7 + 6 = 80$
EDS (Anthracene) $= \{246 + 343 + 350 + 246 + 165 + 170 + 132 + 165 + 170 + 132 + 246 + 350 + 343 + 246\} = 3304$

$$\begin{pmatrix}
0&1&2&3&2&1&2&3&4&3&4&5&6&5\\
1&0&1&2&3&2&3&4&5&4&5&6&7&6\\
2&1&1&1&2&3&4&5&4&3&6&7&6&5\\
3&2&1&0&1&2&3&4&3&2&5&6&5&4\\
2&3&2&1&0&1&2&3&2&1&4&5&4&3\\
1&2&3&2&1&1&1&2&3&2&3&4&5&4\\
2&3&4&3&2&1&0&1&2&3&2&3&4&3\\
3&4&5&4&3&2&1&0&1&2&1&2&3&2\\
4&5&4&3&2&3&2&1&1&1&2&3&2&1\\
3&4&3&2&1&2&3&2&1&0&3&4&3&2\\
4&5&6&5&4&3&2&3&2&3&0&1&2&3\\
5&6&7&6&5&4&3&2&3&4&1&1&1&2\\
6&7&6&5&4&5&4&3&2&3&2&1&0&1\\
5&6&5&4&3&4&3&2&1&2&3&2&1&0
\end{pmatrix}$$

2.4 Molecular Graph of Tetracene

The structure of tetracene consists of 18 vertices. Here, 12 vertices are of degree 2 and six vertices are of degree 3 (Fig. 4 and Table 4).

Minimum Dominating Distance Matrix (18 × 18) of Tetracene

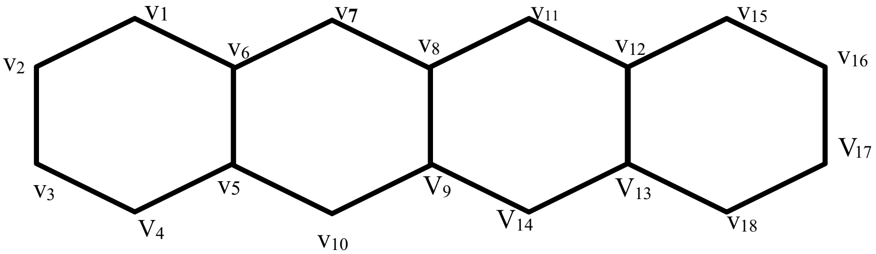

Fig. 4 Tetracene

Table 4 Eccentricity of molecular graph of Tetracene

$e(v_1)$	8
$e(v_2)$	9
$e(v_3)$	9
$e(v_4)$	8
$e(v_5)$	7
$e(v_6)$	7
$e(v_7)$	6
$e(v_8)$	5
$e(v_9)$	5
$e(v_{10})$	6
$e(v_{11})$	6
$e(v_{12})$	7
$e(v_{13})$	7
$e(v_{14})$	6
$e(v_{15})$	8
$e(v_{16})$	9
$e(v_{17})$	9
$e(v_{18})$	8

TE (Tetracene) = 8 + 9 + 9 + 8 + 7 + 7 + 6 + 5 + 5 + 6 + 6 + 7 + 7 + 6 + 8 + 9 + 9 + 8 = 130
EDS (Tetracene) = 8514

$$\begin{pmatrix}
0&1&2&3&2&1&2&3&4&3&4&5&6&5&6&7&8&7\\
1&0&1&2&3&2&3&4&5&4&5&6&7&6&7&8&9&8\\
2&1&1&1&2&3&4&5&4&3&6&7&6&5&8&9&8&7\\
3&2&1&0&1&2&3&4&3&2&5&6&5&4&7&8&7&6\\
2&3&2&1&0&1&2&3&2&1&4&5&4&3&6&7&6&5\\
1&2&3&2&1&1&1&2&3&2&3&4&5&4&5&6&7&6\\
2&3&4&3&2&1&0&1&2&3&2&3&4&3&4&5&6&5\\
3&4&5&4&3&2&1&0&1&2&1&2&3&2&3&4&5&4\\
4&5&4&3&2&3&2&1&1&1&2&3&2&1&4&5&4&3\\
3&4&3&2&1&2&3&2&1&0&3&4&3&2&5&6&5&4\\
4&5&6&5&4&3&2&1&2&3&0&1&2&3&2&3&4&3\\
5&6&7&6&5&4&3&2&3&4&1&1&1&2&1&2&3&2\\
6&7&6&5&4&5&4&3&2&3&2&1&0&1&2&3&2&1\\
5&6&5&4&3&4&3&2&1&2&3&2&1&0&3&4&3&2\\
6&7&8&7&6&5&4&3&4&5&2&1&2&3&0&1&2&3\\
7&8&9&8&7&6&5&4&5&6&3&2&3&4&1&0&1&2\\
8&9&8&7&6&7&6&5&4&5&4&3&2&3&2&1&1&1\\
7&8&7&6&5&6&7&4&3&4&3&2&1&2&3&2&1&0
\end{pmatrix}$$

2.5 Molecular Graph of Pentacene

The structure of tetracene consists of 22 vertices. Here 12 vertices are of degree 2 and ten vertices are of degree 3 (Fig. 5 and Table 5).

Minimum Dominating Distance Matrix (22 × 22) of Pentacene

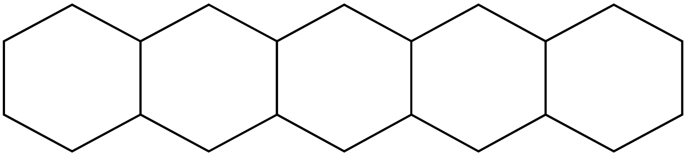

Fig. 5 Pentacene

Table 5 Eccentricity of molecular graph of Pentacene

$e(v_1)$	10
$e(v_2)$	11
$e(v_3)$	11
$e(v_4)$	10
$e(v_5)$	9
$e(v_6)$	9
$e(v_7)$	8
$e(v_8)$	7
$e(v_9)$	7
$e(v_{10})$	8
$e(v_{11})$	6
$e(v_{12})$	7
$e(v_{13})$	7
$e(v_{14})$	6
$e(v_{15})$	8
$e(v_{16})$	9
$e(v_{17})$	9
$e(v_{18})$	8
$e(v_{19})$	10
$e(v_{20})$	11
$e(v_{21})$	11
$e(v_{22})$	10

TE (Pentacene) = {10 + 11 + 11 + 10 + 9 + 9 + 8 + 7 + 7 + 8 + 6 + 7 + 7 + 6 + 8 + 9 + 9 + 8 + 10 + 11 + 11 + 10} = 192

EDS (Pentacene) = 18,280

$$
\begin{pmatrix}
0 & 1 & 2 & 3 & 2 & 1 & 2 & 3 & 4 & 3 & 4 & 5 & 6 & 5 & 6 & 7 & 8 & 7 & 8 & 9 & 10 & 9 \\
1 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 5 & 4 & 5 & 6 & 7 & 6 & 7 & 8 & 9 & 8 & 9 & 10 & 11 & 10 \\
2 & 1 & 1 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 6 & 7 & 6 & 5 & 8 & 9 & 8 & 7 & 10 & 11 & 10 & 9 \\
3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 & 2 & 5 & 6 & 5 & 4 & 7 & 8 & 7 & 6 & 9 & 10 & 9 & 8 \\
2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 1 & 4 & 5 & 4 & 3 & 6 & 7 & 6 & 5 & 8 & 9 & 8 & 7 \\
1 & 2 & 3 & 2 & 1 & 1 & 1 & 2 & 3 & 2 & 3 & 4 & 5 & 4 & 5 & 6 & 7 & 6 & 7 & 8 & 9 & 8 \\
2 & 3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 3 & 4 & 5 & 6 & 5 & 6 & 7 & 8 & 7 \\
3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 1 & 2 & 3 & 2 & 3 & 4 & 5 & 4 & 5 & 6 & 7 & 6 \\
4 & 5 & 4 & 3 & 2 & 3 & 2 & 1 & 1 & 1 & 2 & 3 & 2 & 1 & 4 & 5 & 4 & 3 & 6 & 7 & 6 & 5 \\
3 & 4 & 3 & 2 & 1 & 2 & 3 & 2 & 1 & 0 & 3 & 4 & 3 & 2 & 5 & 6 & 5 & 4 & 7 & 8 & 7 & 6 \\
4 & 5 & 6 & 5 & 4 & 3 & 2 & 1 & 2 & 3 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 3 & 4 & 5 & 6 & 5 \\
5 & 6 & 7 & 6 & 5 & 4 & 3 & 2 & 3 & 4 & 1 & 1 & 1 & 2 & 1 & 2 & 3 & 2 & 3 & 4 & 5 & 4 \\
6 & 7 & 6 & 5 & 4 & 5 & 4 & 3 & 2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 1 & 4 & 3 & 4 & 3 \\
5 & 6 & 5 & 4 & 3 & 4 & 5 & 2 & 1 & 2 & 3 & 2 & 1 & 0 & 3 & 4 & 3 & 2 & 5 & 6 & 5 & 4 \\
6 & 7 & 8 & 7 & 6 & 5 & 4 & 3 & 4 & 3 & 2 & 1 & 2 & 3 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 3 \\
7 & 8 & 9 & 8 & 7 & 6 & 5 & 4 & 5 & 4 & 3 & 2 & 3 & 4 & 1 & 0 & 1 & 2 & 1 & 2 & 3 & 2 \\
8 & 9 & 8 & 7 & 6 & 7 & 6 & 5 & 4 & 5 & 4 & 3 & 2 & 3 & 2 & 1 & 1 & 1 & 2 & 3 & 2 & 1 \\
7 & 8 & 7 & 6 & 5 & 6 & 7 & 4 & 3 & 4 & 3 & 2 & 1 & 2 & 3 & 2 & 1 & 0 & 3 & 4 & 3 & 2 \\
8 & 9 & 10 & 9 & 8 & 7 & 6 & 5 & 6 & 7 & 4 & 3 & 4 & 5 & 2 & 1 & 2 & 3 & 0 & 1 & 2 & 3 \\
9 & 10 & 11 & 10 & 9 & 8 & 7 & 6 & 7 & 8 & 5 & 4 & 3 & 6 & 3 & 2 & 3 & 4 & 1 & 1 & 1 & 2 \\
10 & 11 & 10 & 9 & 8 & 9 & 8 & 7 & 6 & 7 & 6 & 5 & 4 & 5 & 4 & 3 & 2 & 3 & 2 & 1 & 0 & 1 \\
9 & 10 & 9 & 8 & 7 & 8 & 7 & 6 & 5 & 6 & 5 & 4 & 3 & 4 & 3 & 2 & 1 & 2 & 3 & 2 & 1 & 0
\end{pmatrix}
$$

Problem: For the Molecular Graph of Linear Benzenoid system, The Total Eccentricty of Linear Benzenoid System (LBS) for $h \leq 5$ hexagons can be defined as TE (LBS(h)) = (1/12)*($h^4 - 14h^3 + 143\text{h}^2 - 58h + 144$).

Solution

Consider linear benzenoid system LBS (h) with h hexagons.

Using the definition of total eccentricity and using the method of computations (2.1, 2.2, 2.3, 2.4, 2.5).

Total eccentricity of the molecular graph of benzene = 18.

Total eccentricity of the molecular graph of naphthalene = 42.

Total eccentricity of the molecular graph of anthracene = 80.

Total eccentricity of the molecular graph of tetracene = 130.

Total eccentricity of the molecular graph of pentacene = 192.

Let us take x as hexagons and y as the total eccentricity of the molecular graph of linear benzenoid system LBS(h) with the corresponding hexagons, respectively.

We form forward difference table (Table 6).

Forward difference table

x	y	Δy	Δy²	Δy³	Δy⁴
1	18				
2	42	24			
3	80	38	14		
4	130	50	12	-2	
5	192	62	12	0	2

From the above table, using Newton's forward interpolation formula [13], we get, $y = (1/12)*(x^4 - 14x^3 + 143x^2 - 58x + 144)$.

Now the molecular graph of benzene, naphthalene, anthracene, tetracene and pentacene contains 1, 2, 3, 4 and 5 hexagons, respectively.

Here we can consider hexagon $h = x$.

Molecular graph of linear benzenoid system contains h hexagons.

So, we can conclude that the total eccentricty of linear benzenoid system (LBS) for h hexagons is TE (LBS(h)) $= (1/12)*(h^4 - 14h^3 + 143h^2 - 58h + 144)$ where $h \leq 5$.

3 Conclusion

In this paper, eccentric distance sum in the graph of chemical compounds that depends on minimum dominating distance matrix is shown and then total eccentricity of linear benzenoid system (LBS) for h hexagons where $h \leq 5$ is computed. Aim of this paper is to present the importance of graph theoretical ideas in chemical structure for researches. This paper obtains a new approach associated with the molecular graph using domination concepts.

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