Some Topological Indices of Tetrameric 1,3-Adamantane

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ABSTRACT

Topological indices are numerical parameters of a graph which characterize its topology. In this paper the PI, Szeged and Zagreb group indices of the tetrameric 1,3-adamantane are computed.

Keywords: PI index, Szeged index, Zagreb index, tetrameric 1,3-adamatane.

1. INTRODUCTION

Diamondoids are an important class of organic compounds with unique structures and properties. This family of compounds with over 20000 variants is one of the best candidates for molecular building blocks (MBBs) to construct nanostructures compared to other MBBs known so far, Figure 1.

Let G be a simple molecular graph with vertex and edge sets V(G) and E(G), respectively. As usual, the distance between the vertices u and v of G is denoted by $d_G(u,v)$ (or d(u,v) for short) and it is defined as the number of edges in a minimal path connecting vertices u and v.[3]

The first and second Zagreb indices, as well as the first Geometric-Arithmetic indices of a graph G are defined as:

$$M_1(G) = \Sigma_{e=uv}[d(u)+d(v)],\ M_2(G) = \Sigma_{e=uv}[d(u)d(v)],\ GA_1(G) = \sum_{e=uv}\frac{2\sqrt{d(u)d(v)}}{[d(u)+d(v)]},$$

where d(u) is the degree of the vertex u and d(v) is defined analogously.[1-3,10]

The eccentric connectivity index of the graph G is defined as: $\xi(G) = \sum_{u\epsilon V(G)} \deg(u).\varepsilon(u)$ where $\varepsilon(u) = \max\{d(u,x) : x\epsilon V(G)\}$.[4-6]

The vertex PI, Szeged and second Geometric-Arithmetic indices of a graph G are defined as $PI_v(G) = \Sigma_{e=uv}[n_u(e) + n_v(e)]$, $Sz(G) = \Sigma_{e=uv}[n_u(e)n_v(e)]$ and $GA_2(G) = \sum_{e=uv}\frac{2\sqrt{n_u(e)n_v(e)}}{[n_u(e)+n_v(e)]}$, where $n_u(e)$ is the number of vertices lying closer to u than to v and $n_v(e)$ is defined analogously.[7-10]

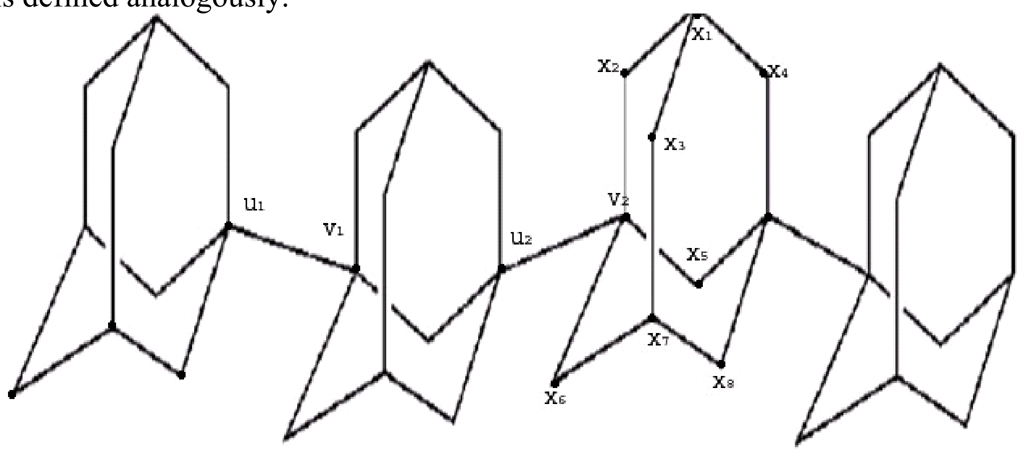

Figure 1. The tetrameric 1,3-adamantane(TA[4]).

The PI, edge Szeged and third Geometric-Arithmetic indices of a graph G are defined as $PI(G) = \Sigma_{e=uv}[m_u(e)+m_v(e)]$, $Sz_e(G) = \Sigma_{e=uv}[m_u(e)m_v(e)]$ and $GA_3(G) = \sum_{e=uv}\frac{2\sqrt{m_u(e)m_v(e)}}{[m_u(e)+m_v(e)]}$, where $m_u(e)$ is the number of edges lying closer to u than to v and $m_v(e)$ is defined analogously.[10-20] The mathematical properties of these topological indices can be found in some recent papers.[21-22]

In this paper our notation is standard and taken mainly from the standard book of graph theory.

2. ZAGREB GROUP, GA_1 AND ECCENTRIC CONNECTIVITY INDICES OF TA[N]

By simple calculations one can see that, $|V(TA[n])| = 10n$ and $|E(TA[n])| = 13n - 1$. We now compute the Zagreb group and GA_1 indices of TA[n]. We begin by the first and second Zagreb index.

$$\begin{aligned} M_1(TA[n]) &= \sum_{e=uv}\big(d(u) + d(v)\big) \\ &= 2[9(3+2) + 3(4+2)] + (n-2)[6(3+2) + 6(4+2)] + (n-1)(4+4) \\ &= 74n - 14, \end{aligned}$$

$$\begin{aligned} M_1(TA[n]) &= \sum_{e=uv}[d(u) \times d(v)] \\ &= 2[9(3\times 2) + 3(4\times 2)] + (n-2)[6(3\times 2) + 6(4\times 2)] + 16(n-1) \\ &= 100n - 28. \end{aligned}$$

Lemma 1. $GA_1(TA[n]) = \left(\frac{12\sqrt{6}}{5} + 4\sqrt{2} + 1\right)n + \frac{12\sqrt{6}}{5} - 4\sqrt{2} - 1.$

Proof. By definition,

$$\begin{aligned} GA_1(TA[n]) &= \sum_{e=uv}\frac{2\sqrt{du.dv}}{du+dv} \\ &= 2\left[2\left(9\times\frac{\sqrt{6}}{5} + 3\times\frac{\sqrt{8}}{6}\right) + (n-2)\left(6\times\frac{\sqrt{6}}{5} + 6\times\frac{\sqrt{8}}{6}\right) + \frac{1}{2}(n-1)\right] \\ &= \left(\frac{12\sqrt{6}}{5} + 4\sqrt{2} + 1\right)n + \frac{12\sqrt{6}}{5} - 4\sqrt{2} - 1. \end{aligned}$$

□

Theorem 2. $\xi(TA[n]) = \begin{cases} 58.5n^2 + 25n & \text{if n is even} \\ 59n^2 + 64n + 8 & \text{if n is odd} \end{cases}.$

Proof. If n is even then for k^th copy of TA[1], $2 \le k \le \frac{n}{2}$, in the molecular graph of TA[n], we have

$$\begin{aligned} \varepsilon(x_1) = \varepsilon(x_7) = \varepsilon(v_{k-1}) &= 3 + 2(n-k-1) + (n-k) + 2, \\ \varepsilon(x_2) = \varepsilon(x_3) = \varepsilon(x_6) &= 3 + 2(n-k-1) + (n-k) + 3, \\ \varepsilon(x_4) = \varepsilon(x_5) = \varepsilon(x_8) &= 3 + 2(n-k-1) + (n-k) + 1, \\ &\vdots \\ \varepsilon(u_k) &= 3 + 2(n-k-1) + (n-k). \end{aligned}$$

Thus for this copy of TA[1], $\sum_{u\varepsilon V(TA[1])} \deg(u)\,\varepsilon(u) = 78\,n + 78\,k + 70$. For k^th copy of TA[1], $\frac{n}{2} + 1 \le k \le n-1$, in definition of TA[n] the value is equal to $78\,n + 78\,k + 70$. Therefore,

$$\begin{aligned} \xi(TA[n]) &= \sum_{u\epsilon V(G)} \deg(u)\,.\,\varepsilon(u) \\ &= 2\sum_{k=2}^{\frac{n}{2}}(78\,n - 78\,k + 70) \\ &\quad + 2[27\,n + 6(3\,n+1) + 6(3\,n-1) + 4(3\,n-2)] \\ &= (58.5n^2 - 125\,n + 16) + (150\,n - 16) \\ &= 58.5\,n^2 + 25\,n. \end{aligned}$$

If n is odd then for $k = \left[\frac{n}{2}\right] + 1$, we have:

$$\varepsilon(x_1) = \varepsilon(x_7) = \varepsilon(v_{k-1}) = \varepsilon(u_k) = 3 + 2(n-k-1) + (n-k) + 2$$

$\varepsilon(x_2) = \varepsilon(x_3) = \varepsilon(x_4) = \varepsilon(x_6) = \varepsilon(x_8) = 3 + 2(n-k-1) + (n-k) + 3$
$\varepsilon(x_5) = 3 + 2(n-k-1) + (n-k) + 1.$

Therefore

$$\xi(TA[n]) = \sum_{u \in V(G)} \deg(u) \cdot \varepsilon(u)$$
$$= 2\sum_{k=2}^{\frac{n}{2}} (78n - 78k + 70) + \left(78n - 78\left(\left[\frac{n}{2}\right] + 1\right) + 86\right) + (150n - 16)$$
$$= 156n\left[\frac{n}{2}\right] - 78\left[\frac{n}{2}\right]^2 - 16\left[\frac{n}{2}\right] + 72n + 8$$
$$= 59n^2 + 64n + 8.$$

The proof is complete. □

3. THE VERTEX PI, SZEGED AND GA2 INDEX OF TA[N].

In this section the vertex PI, Szeged and GA_2 indices of the tetrameric 1,3-adamantane, TA[n], are computed. If A and B are graphs such that $V(A) \subseteq V(B)$ and $E(A) \subseteq E(B)$ then A is called a subgraph of B, $A \leq B$. To compute these topological indices, we partition the edge set of TA[n] into the classes with the same $n_u(e)$ and $n_v(e)$, where $e = uv$ is an edge of TA[n]. We first notice that the graph TA[n] can be constructed from subgraphs isomorphic to TA[1] and the edges between them, see Figure 1 and 2.

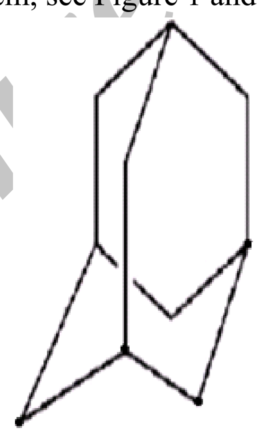

Figure 2. TA[1].

We can see $n_u(e) + n_v(e) = 10n$ for e in E(TA[n]), thus $PIv(TA[n]) = 10n \times (13n - 1) = 130n^2 - 10n$.

Theorem 3. $Sz\,(TA[n]) = \frac{350}{3}n^3 + 240n^2 - \frac{206}{3}n$.

Proof. We partition the edges TA[n] in two ways, the edges between two copies of TA[1] and the edges copy of TA[1](figure 1). If $e = u_i v_i$ thus $n_{u_i}(e) = 10i$ and $n_{v_i}(e) =$

$10(n-i)$. For k[th] copy of TA[1], if $e = uv = x_1x_2, u_kx_5, x_6x_7$ then $n_u(e) = 10(n-k)+6$ and $n_v(e) = 10(k-1)+4$. If $e = uv = x_1x_4, v_{k-1}x_5, x_7x_8$ then $n_u(e)$ and $n_v(e)$ are as above. For $e = x_1x_3, x_2v_{k-1}, v_{k-1}x_6, x_4u_k, u_kx_8, x_3x_7$ we have $n_u(e) = 10(n-1)+6$ and $n_v(e) = 4$.
Therefore

$$
\begin{aligned}
Sz\,(TA[n]) &= \sum_{e=uv\epsilon E(TA[n])} \left(n_u(e)n_v(e)\right) \\
&= 100\sum_{i=1}^{n-1} i(n-i) \\
&+ 3\sum_{k=1}^{n}(10(n-k)+6)(10(k-1)+4) \\
&+ 3\sum_{k=1}^{n}(10(n-k)+4)(10(k-1)+6) \\
&+6\sum_{k=1}^{n}4(6+10(n-1)) \\
&= \frac{50}{3}(n^3-n) + 100\,n^3 + 240\,n^2 - 52\,n \\
&= \frac{350}{3}n^3 + 240\,n^2 - \frac{206}{3}n.
\end{aligned}
$$
□

Theorem 4. $GA_2\,(TA[n]) \le n - 1 + 1.2\sqrt{25\,n^2-1} + 2.4\sqrt{10\,n-4}$.

Proof. By above calculation

$$
\begin{aligned}
GA_2\,(TA[n]) &= \sum_{e=uv}\frac{2\sqrt{n_u(e)n_v(e)}}{n_u(e)+n_v(e)} \\
&= \frac{2}{n}\sum_{i=1}^{n-1}\sqrt{ni-i^2} + \frac{3}{5n}\sum_{k=1}^{n}\sqrt{(10n-10k+6)(10k-6)} \\
&+ \frac{3}{5n}\sum_{k=1}^{n}\sqrt{(10n-10k+4)(10k-4)} + \frac{12}{5}\sqrt{10\,n-4}.
\end{aligned}
$$

Thus by Cauchy-Schwarz Inequality we have

$$GA_2\,(TA[n]) \le n - 1 + 1.2\sqrt{25\,n^2-1} + 2.4\sqrt{10\,n-4}.$$
□

4. The PI, edge Szeged and third Geometric-Arithmetic Index of TA[N].

The aim of this section is to compute The PI, edge Szeged and third GA index of TA[n].

Theorem 5. $PI(TA[n]) = 169n^2 - 63n + 2$ and $Sz_e(TA[n]) = 169n^3 + 65n^2 - 17n - 1 + (169/6)(n^3 - n)$.

Proof. By definition, if $e = u_i v_i$ then $m_{u_i}(e) = 13i - 1$ and $m_{v_i}(e) = 13(n - i) - 1$. For $e = uv = x_1x_2, x_5u_k, x_6x_7$ we have $m_u(e) = 6 + 13(n-k)$ and $m_v(e) = 3 + 13(k-1)$ and for $e = uv = x_1x_4, v_{k-1}x_5, x_7x_8$, $m_u(e) = 6 + 13(k-1)$ and $m_v(e) = 3 + 13(n-k)$. If $e = uv = x_2v_{k-1}, x_3x_7, x_4u_k$ then $m_u(e) = 3$ and $m_v(e) = 6 + 13(n-k) + 13(k-1)$ and also for $e = uv = x_1x_3, u_kx_8, v_{k-1}x_6$ we can see $m_u(e) = 6 + 13(n-k) + 13(k-1)$ and $m_v(e) = 3$. Therefore

$$\begin{aligned}
PI(TA[n]) &= \sum_{e=uv} \big(m_u(e) + m_v(e)\big) \\
&= \sum_{i=1}^{n-1} \big((13i - 1) + 13(n-i) - 1\big) \\
&+ 12\sum_{k=1}^{n} (9 + 13(n-k) + 13(k-1)) \\
&= (n-1)(13n-2) + 12(13n-4) \\
&= 169n^2 - 63n + 2.
\end{aligned}$$

Also by similar argument

$$\begin{aligned}
Sz_e(TA[n]) &= \sum_{e=uv} \big(m_u(e)m_v(e)\big) \\
&= \sum_{i=1}^{n-1}(13i-1)(13n-13i-1) + 3\sum_{k=1}^{n}\big(6 + 13(n-k)\big)(3 + 13(k-1)) \\
&+ 3\sum_{k=1}^{n}\big(6 + 13(k-1)\big)(3 + 13(n-k)) + 18\sum_{k=1}^{n}(6 + 13(n-k) + 13(k-1)) \\
&= 169n^3 + 65n^2 - 17n - 1 + \frac{169}{6}(n^3 - n).
\end{aligned}$$

□

Theorem 6. $GA_3(TA[n]) \le \frac{1}{13n-2}(13n^2 - 15n + 2) + \frac{6n}{13n-4}\sqrt{169n^2 - 104n + 7} + \frac{12n}{13n-4}\sqrt{39n - 21}.$

Proof. By definition of GA_3 index and the computation of Theorem 5,

$$\begin{aligned}
GA_3(TA[n]) &= \sum_{e=uv} \frac{2\sqrt{m_u(e)m_v(e)}}{m_u(e) + m_v(e)} \\
&= \frac{2}{13n-2}\sum_{i=1}^{n-1}\sqrt{(13i-1)(13n-13i-1)} \\
&+ \frac{6}{13n-4}\sum_{k=1}^{n}\sqrt{(13n-13k+6)(13k-10)} \\
&+ \frac{6}{13n-4}\sum_{k=1}^{n}\sqrt{(13n-13k+3)(13k-7)} \\
&+ \frac{12n}{13n-4}\sqrt{3(13n-7)}.
\end{aligned}$$

Therefore by Cauchy-Schwarz Inequality, we have

$$GA_3\ (TA[n])\ \leq \frac{1}{13n-2}(13n^2-15n+2) + \frac{6n}{13n-4}\sqrt{169\,n^2-104n+7} + \frac{12n}{13n-4}\sqrt{39\,n-21}.$$

This complete the proof. □

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