

Original Article

# Molecular Structures of the Tadpole Graph using Alpha and Gamma Indices

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Received: 27 May 2025

Revised: 30 June 2025

Accepted: 19 July 2025

Published: 29 July 2025

**Abstract** - The sum of the squares of the degrees of the vertices multiplied by the number of edges incident to each vertex is called Alpha Gourava Indices and the sum of the cubes of the degrees of the vertices is called Gamma Gourava Indices. In these paper, we compute the molecular structure of the Tadpole graph using the Alpha and Gamma Gourava Indices.

**Keywords** - Alpha Gourava Indices, Gamma Gourava Indices, Tadpole graph.

## 1. Introduction

Let  $G$  be a simple, finite, connected graph with the vertex set  $V(G)$  and edge set  $E(G)$ . The degree  $d_G(u)$  of a vertex  $u$  is the number of vertices adjacent to  $u$ . The additional definitions and notations, the reader may refer to [1]. A molecular graph is a graph in which the vertices correspond to the atoms and the edges to the bonds of a molecule. A topological index is a numeric quantity from structural graph of a molecule. Several topological indices have been considered in Theoretical Chemistry, and have found some applications, especially in QSPR/QSAR study, see [2, 3, 4]. In Chemical Science, numerous vertex degree based topological indices or graph indices have been introduced and extensively studied in [4, 5].

The first and second Gourava indices [6] of a graph  $G$  are defined as follows

$$GO_1(G) = \sum_{uv \in E(G)} [d_u + d_v + d_u d_v]$$

$$\begin{aligned} GO_2(G) &= \sum_{uv \in E(G)} (d_u + d_v)(d_u d_v) \\ &= \sum_{uv \in E(G)} (d_u^2 d_v + d_u d_v^2) \end{aligned}$$

The first and second Alpha Gourava indices [6] of a graph  $G$  are defined as follows

$$AG O_1(G) = \sum_{uv \in E(G)} [d_u^2 + d_v^2 + d_u d_v]$$

$$\begin{aligned} AG O_2(G) &= \sum_{uv \in E(G)} (d_u^2 + d_v^2)(d_u d_v) \\ &= \sum_{uv \in E(G)} (d_u^3 d_v + d_u d_v^3) \end{aligned}$$

The first and second Gamma Gourava indices [6] of a graph  $G$  are defined as follows.

$$\begin{aligned} GG O_1(G) &= \sum_{uv \in E(G)} [d_u^3 + d_v^3 + d_u d_v] \\ GG O_2(G) &= \sum_{uv \in E(G)} (d_u^3 + d_v^3)(d_u d_v) \\ &= \sum_{uv \in E(G)} (d_u^4 d_v + d_u d_v^4) \end{aligned}$$

## 2. Results for Tadpole Graph

$T_{m,n}$  denotes the tadpole graph constructed by joining a cycle  $C_m$  to a path  $P_n$ . Where  $m \geq 3$  and  $n \geq 1$ . Tadpole graph is also called as dragon graph.



Generally, in  $G$ , vertex set can be denoted as  $V(G)$  and set of all edges represents  $E(G)$  respectively. Also, the number of vertices  $|V(G)| = m + n$  and number of edges  $|E(G)| = m + n$ .

The Tadpole graph have two cases

**Case 1:**  $T_{m,n}$  where  $m \geq 3$  and  $n = 1$

**Case 2:**  $T_{m,n}$  where  $m \geq 3$  and  $n > 1$

**Case 1:** Vertex and edge partition of tadpole graphs  $T_{m,n}$  where  $m \geq 3$  and  $n = 1$

We split  $V(G)$  into three subsets  $V_1, V_2$  &  $V_3$  as the following three partitions.

$$\begin{aligned} V_1 &= \{v \in V(G); d_G(v) = 1\}; |V_1| = 1 \\ V_2 &= \{v \in V(G); d_G(v) = 2\}; |V_2| = m - 1, \text{ and} \\ V_3 &= \{v \in V(G); d_G(v) = 3\}; |V_3| = 1 \end{aligned}$$

Similarly, we consider the partition of edge set  $E(G)$  of  $G$  as  $E_{2,2}, E_{3,1}$  &  $E_{3,2}$ . That is,

$$\begin{aligned} E_{2,2} &= \{uv \in E(G): d_G(u) = d_G(v) = 2\}; |E_1| = m - 2. \\ E_{3,2} &= \{uv \in E(G): d_G(u) = 3, d_G(v) = 2\}; |E_2| = 2. \\ E_{3,1} &= \{uv \in E(G): d_G(u) = 3, d_G(v) = 1\}; |E_3| = 1. \end{aligned}$$

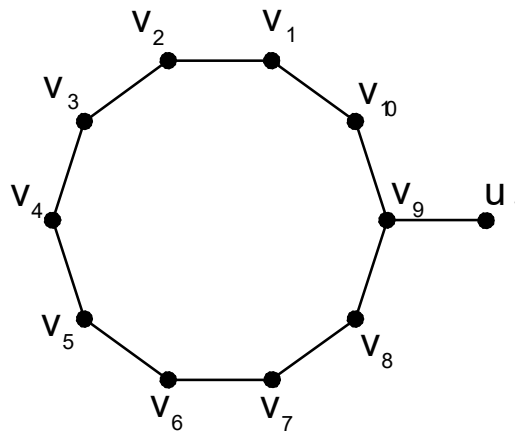


Fig. 1  $T_{10,1}$  graph

**Case 2:** Vertex and edge partition of tadpole graphs  $T_{m,n}$  where  $m \geq 3$  and  $n > 1$  is considered below.

In this case we split  $V(G)$  into three subsets  $V_1, V_2$  &  $V_3$  as the following three partitions.

$$\begin{aligned} V_1 &= \{v \in V(G); d_G(v) = 1\}; |V_1| = 1 \\ V_2 &= \{v \in V(G); d_G(v) = 2\}; |V_2| = m + n - 2, \text{ and} \\ V_3 &= \{v \in V(G); d_G(v) = 3\}; |V_3| = 1 \end{aligned}$$

Similarly, we consider the partition of edge set  $E(G)$  of  $G$  as  $E_{2,1}, E_{2,2}$  &  $E_{2,3}$ . That is,

$$\begin{aligned} E_{2,2} &= \{uv \in E(G): d_G(u) = d_G(v) = 2\}; |E_1| = m + n - 4. \\ E_{2,3} &= \{uv \in E(G): d_G(u) = 3, d_G(v) = 2\}; |E_2| = 3. \\ E_{2,1} &= \{uv \in E(G): d_G(u) = 2, d_G(v) = 1\}; |E_3| = 1. \end{aligned}$$

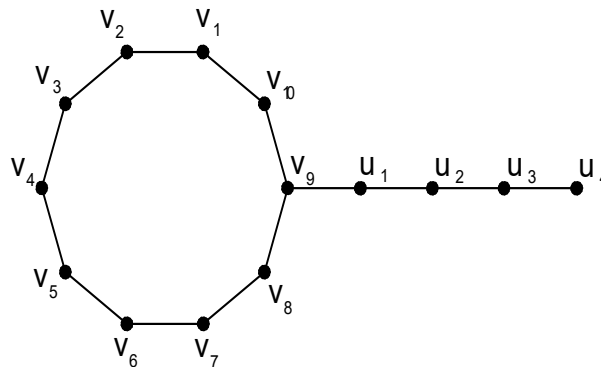


Fig. 2  $T_{10,4}$  Graph

**Theorem 2.1:** The first and second Gourava indices of a Tadpole graph are

$$GO_1(T_{(m,n)}) = 8m + 13 \text{ where } m \geq 3 \text{ and } n = 1$$

$$GO_2(T_{(m,n)}) = 16m + 40 \text{ where } m \geq 3 \text{ and } n = 1$$

**Proof:** Let  $G = T_{m,n}$  be a tadpole graph. Let the vertex set  $V(G) = \{v_1, v_2, \dots, v_n\} \cup \{u_1, u_2, \dots, u_n\}$ . Where  $v_i \in V(C_m)$  and  $u_i \in P_n$ .

We have,

$$\begin{aligned} GO_1(T_{m,n}) &= \sum_{v_1 v_2 \in E(G)} [d_u + d_v + d_u d_v] \\ &= \sum_{E_1} [d_2(v_1) + d_2(v_2) + d_1(v_1)d_2(v_2)] + \sum_{E_2} [d_3(v_1) + d_2(v_2) + \\ &\quad d_3(v_1)d_2(v_2)] + \sum_{E_3} [d_3(v_1) + d_1(v_2) + d_3(v_1)d_1(v_2)] \\ &= (m-2)8 + 2 \times 11 + 1 \times 7 \\ GO_1(T_{m,n}) &= 8m + 13 \\ GO_2(G) &= \sum_{uv \in E(G)} (d_u^2 d_v + d_u d_v^2) \\ &= \sum_{uv \in E(G)} (d_2^2(v_1)d_2(v_2) + d_2(v_1)d_2^2(v_2)) + \\ &\quad \sum_{uv \in E(G)} (d_3^2(v_1)d_2(v_2) + d_3(v_1)d_2^2(v_2)) + \\ &\quad \sum_{uv \in E(G)} (d_3^2(v_1)d_1(v_2) + d_3(v_1)d_1^2(v_2)) \\ &= (m-2) \times 16 + 2 \times 30 + 12 \\ &= 16m + 40 \end{aligned}$$

**Theorem 2.2:** The first and second Gourava indices of a Tadpole graph are

$$GO_1(T_{(m,n)}) = 8m + 8n + 6 \text{ where } m \geq 3 \text{ and } n > 1$$

$$GO_2(T_{(m,n)}) = 16m + 16n + 32 \text{ where } m \geq 3 \text{ and } n > 1$$

**Proof:** Let  $G = T_{m,n}$  be a tadpole graph. Let the vertex set  $V(G) = \{v_1, v_2, \dots, v_n\} \cup \{u_1, u_2, \dots, u_n\}$ . Where  $v_i \in V(C_m)$  and  $u_i \in P_n$ .

We have,

$$\begin{aligned} GO_1(T_{m,n}) &= \sum_{v_1 v_2 \in E(G)} [d_u + d_v + d_u d_v] \\ &= \sum_{E_1} [d_2(v_1) + d_2(v_2) + d_2(v_1)d_2(v_2)] + \sum_{E_2} [d_3(v_1) + d_2(v_2) + \\ &\quad d_3(v_1)d_2(v_2)] + \sum_{E_3} [d_2(v_1) + d_1(v_2) + d_2(v_1)d_1(v_2)] \\ &= (m+n-4)8 + 3 \times 11 + 5 \\ GO_1(T_{m,n}) &= 8m + 8n + 6 \\ GO_2(G) &= \sum_{uv \in E(G)} (d_u^2 d_v + d_u d_v^2) \\ &= \sum_{uv \in E(G)} (d_2^2(v_1)d_2(v_2) + d_2(v_1)d_2^2(v_2)) + \\ &\quad \sum_{uv \in E(G)} (d_3^2(v_1)d_2(v_2) + d_3(v_1)d_2^2(v_2)) + \\ &\quad \sum_{uv \in E(G)} (d_2^2(v_1)d_1(v_2) + d_2(v_1)d_1^2(v_2)) + \\ &= (m+n-4) \times 16 + 3 \times 30 + 6 \\ &= 16m + 16n + 32 \end{aligned}$$

**Theorem 2.3:** The first and second Alpha Gourava indices of a Tadpole graph are

$$AG O_1(T_{(m,n)}) = 3(4m + 9) \text{ where } m \geq 3 \text{ and } n = 1$$

$$AG O_2(T_{(m,n)}) = 16m + 40 \text{ where } m \geq 3 \text{ and } n = 1$$

**Proof:** Let  $G = T_{m,n}$  be a tadpole graph. Let the vertex set  $V(G) = \{v_1, v_2, \dots, v_n\} \cup \{u_1, u_2, \dots, u_n\}$ . Where  $v_i \in V(C_m)$  and  $u_i \in P_n$ .

We have,

$$\begin{aligned} AG O_1(G) &= \sum_{uv \in E(G)} [d_u^2 + d_v^2 + d_u d_v] \\ &= \sum_{E_1} [d_2^2(v_1) + d_2^2(v_2) + d_2(v_1)d_2(v_2)] + \sum_{E_2} [d_3^2(v_1) + d_2^2(v_2) + \\ &\quad d_3(v_1)d_2(v_2)] + \sum_{E_3} [d_3^2(v_1) + d_1^2(v_2) + d_3(v_1)d_2(v_2)] \\ &= (m-2) \times 12 + 2 \times 19 + 1 \times 13 \end{aligned}$$

$$AG O_1(G) = 3(4m + 9)$$

$$\begin{aligned} AG O_2(G) &= \sum_{uv \in E(G)} (d_u^2 d_v + d_u d_v^2) \\ &= \sum_{E_1} (d_2^2(v_1)d_2(v_2) + d_2(v_1)d_2^2(v_2)) + \end{aligned}$$

$$\begin{aligned}
& \sum_{E_2} (d_3^2(v_1)d_2(v_2) + d_3(v_1)d_2^2(v_2)) + \\
& \sum_{E_3} (d_3^2(v_1)d_1(v_2) + d_3(v_1)d_1^2(v_2)) \\
& = (m-2) \times 16 + 2 \times 30 + 12 \\
& = 16m + 40
\end{aligned}$$

**Theorem 2.4:** The first and second Alpha Gourava indices of a Tadpole graph are

$$AGO_1(T_{(m,n)}) = 12m + 7 \text{ where } m \geq 3 \text{ and } n > 1$$

$$AGO_2(T_{m,n}) = 32m + 32n + 116 \text{ where } m \geq 3 \text{ and } n > 1$$

**Proof:** Let  $G = T_{m,n}$  be a tadpole graph. Let the vertex set  $V(G) = \{v_1, v_2, \dots, v_n\} \cup \{u_1, u_2, \dots, u_n\}$ . Where  $v_i \in V(C_m)$  and  $u_i \in P_n$ .

We have,

$$\begin{aligned}
AGO_1(G) &= \sum_{uv \in E(G)} [d_u^2 + d_v^2 + d_u d_v] \\
&= \sum_{E_1} [d_2^2(v_1) + d_2^2(v_2) + d_2(v_1)d_2(v_2)] + \sum_{E_2} [d_3^2(v_1) + d_2^2(v_2) + \\
&\quad d_3(v_1)d_2(v_2)] + \sum_{E_3} [d_2^2(v_1) + d_1^2(v_2) + d_2(v_1)d_2(v_2)] \\
&= (m+n-4) \times 12 + 3(13) + 7
\end{aligned}$$

$$AGO_1(G) = 12m + 7$$

Second Alpha Gourava indices

$$\begin{aligned}
AGO_2(G) &= \sum_{uv \in E(G)} (d_u^2 + d_v^2)(d_u d_v) \\
&= \sum_{uv \in E(G)} (d_u^3 d_v + d_u d_v^3) \\
&= \sum_{E_1} (d_2^3(v_1)d_2(v_2) + d_2(v_1)d_2^3(v_2)) + \sum_{E_2} (d_3^3(v_1)d_2(v_2) + d_3(v_1)d_2^3(v_2)) + \\
&\quad \sum_{E_3} (d_2^3(v_1)d_1(v_2) + d_2(v_1)d_1^3(v_2)) \\
&= (m+n-4) \times (32) + 3 \times 78 + 10 \\
&= 32m + 32n + 116
\end{aligned}$$

**Theorem 2.5:** The first and second Gamma Gourava indices of a Tadpole graph are

$$GGO_1(T_{(m,n)}) = 20m + 55 \text{ where } m \geq 3 \text{ and } n = 1$$

$$GGO_2(T_{m,n}) = 64m + 192 \text{ where } m \geq 3 \text{ and } n = 1$$

**Proof:** Let  $G = T_{m,n}$  be a tadpole graph. Let the vertex set  $V(G) = \{v_1, v_2, \dots, v_n\} \cup \{u_1, u_2, \dots, u_n\}$ . Where  $v_i \in V(C_m)$  and  $u_i \in P_n$ .

We have,

$$\begin{aligned}
GGO_1(G) &= \sum_{uv \in E(G)} [d_u^3 + d_v^3 + d_u d_v] \\
&= \sum_{E_1} [d_2^3(v_1) + d_2^3(v_2) + d_2(v_1)d_2(v_2)] + \sum_{E_2} [d_3^3(v_1) + d_2^3(v_2) + \\
&\quad d_3(v_1)d_2(v_2)] + \sum_{E_3} [d_3^3(v_1) + d_1^3(v_2) + d_3(v_1)d_2(v_2)] \\
&= (m-2) \times 12 + 2 \times 19 + 1 \times 13
\end{aligned}$$

$$GGO_1(G) = 20m + 55$$

Second Gamma Gourava indices

$$\begin{aligned}
GGO_2(G) &= \sum_{uv \in E(G)} (d_u^3 + d_v^3)(d_u d_v) \\
&= \sum_{uv \in E(G)} (d_u^4 d_v + d_u d_v^4) \\
&= \sum_{E_1} (d_2^4(v_1)d_2(v_2) + d_2(v_1)d_2^4(v_2)) + \sum_{E_2} (d_3^4(v_1)d_2(v_2) + d_3(v_1)d_2^4(v_2)) + \\
&\quad \sum_{E_3} (d_2^4(v_1)d_1(v_2) + d_2(v_1)d_1^4(v_2)) \\
&= (m-2) \times 64 + 2(210) + 84 \\
&= 64m + 192
\end{aligned}$$

**Theorem 2.6:** The first and second Gamma Gourava indices of a Tadpole graph are

$$GG O_1(T_{(m,n)}) = 20m + 20n + 13 \text{ where } m \geq 3 \text{ and } n > 1$$

$$GG O_2(T_{(m,n)}) = 64m + 64n - 392 \text{ where } m \geq 3 \text{ and } n > 1$$

**Proof:** Let  $G = T_{m,n}$  be a tadpole graph. Let the vertex set  $V(G) = \{v_1, v_2, \dots, v_n\} \cup \{u_1, u_2, \dots, u_n\}$ . Where  $v_i \in V(C_m)$  and  $u_i \in P_n$ .

We have,

$$\begin{aligned} GG O_1(G) &= \sum_{uv \in E(G)} [d_u^3 + d_v^3 + d_u d_v] \\ &= \sum_{E_1} [d_2^3(v_1) + d_2^3(v_2) + d_2(v_1)d_2(v_2)] + \sum_{E_2} [d_3^3(v_1) + d_2^3(v_2) + \\ &\quad d_3(v_1)d_2(v_2)] + \sum_{E_3} [d_3^3(v_1) + d_1^3(v_2) + d_3(v_1)d_2(v_2)] \\ &= (m + n - 4) \times 20 + 3 \times 41 + 1 \times 13 \end{aligned}$$

$$GG O_1(G) = 20m + 20n + 13$$

Second Alpha Gourava indices

$$\begin{aligned} GG O_2(G) &= \sum_{uv \in E(G)} (d_u^3 + d_v^3)(d_u d_v) \\ &= \sum_{uv \in E(G)} (d_u^4 d_v + d_u d_v^4) \\ &= \sum_{E_1} (d_2^4(v_1)d_2(v_2) + d_2(v_1)d_2^4(v_2)) + \sum_{E_2} (d_3^4(v_1)d_2(v_2) + d_3(v_1)d_2^4(v_2)) + \\ &\quad \sum_{E_3} (d_2^4(v_1)d_1(v_2) + d_2(v_1)d_1^4(v_2)) \\ &= (m + n - 4)(64) + 3(210) + 84 \\ &= 64m + 64n - 392 \end{aligned}$$

### 3. Conclusion

First Gourava indices, Alpha Gourava Indices, Gamma Gourava Indices where

$$m \geq 3 \text{ and } n = 1$$

SLNo.	Conditions	Gourava Indices	Alpha Gourava Indices	Gamma Gourava Indices
1	$m \geq 3 \text{ and } n = 1$	$8m + 13$	$3(4m + 9)$	$20m + 55$
2	$m \geq 3 \text{ and } n > 1$	$8m + 8n + 6$	$12m + 7$	$20m + 20n + 13$

First Second indices, Alpha Gourava Indices, Gamma Gourava Indices where

$$m \geq 3 \text{ and } n = 1$$

SLNo.	Conditions	Gourava Indices	Alpha Gourava Indices	Gamma Gourava Indices
1	$m \geq 3 \text{ and } n = 1$	$16m + 40$	$16m + 40$	$64m + 192$
2	$m \geq 3 \text{ and } n > 1$	$16m + 16n + 32$	$32m + 32n + 116$	$64m + 64n - 392$

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