Asia Mathematatika
Volume: 6 Issue: 3 , (2022) Pages: 24 – 28
Available online at **www.asiamath.org**

A note on SDD invariants of clump graphs with Girth size at most three

Paramasivam Murugarajan[1*]
[1]Department of mathematics, Government Arts College(Autonomous)(Affliated to Bharathidasan University), Kumbakonam-612 002,Tamil Nadu, INDIA. Orchid iD: 0000-0002-7947-0325

Received: 04 Nov 2022 • **Accepted:** 07 Dec 2022 • **Published Online:** 30 Dec 2022

Abstract: The symmetric division deg invariant is one of the 200 discrete Adriatic indices introduced several years ago. This SDD invariant has been already proved a valuable invariant in the QSAR(Quantitative Structure Activity Relationship) and QSPR(Quantitative Structure Property Relationship) studies. In this article, we present on exact values of SDD invariants of inorganic Clump graphs with girth size at most three.

Key words: Degree, Zagreb invariant, symmetric division deg invariant

1. Introduction

All the inorganic graphs, unless otherwise specified, are finite, undirected, connected, and simple. Molecular descriptors, being numerical functions of molecular structure, play a prominent role in mathematical chemistry and are used in QSAR and QSPR studies [8] that relate biological or chemical properties of molecules to specific molecular descriptors [3]. Many molecular descriptors are defined as functions of the structure of the underlying molecular graph, such as the Wiener invariant [10], the Zagreb invariant [5] and Balaban invariants [2]. D.Vukicevic et al. proved that many of these descriptors are defined as individual bond contributions. Among the 200 discrete Adriatic invariants studied in [11], whose predictive properties were evaluated against the benchmark datasets of the International Academy of Mathematical Chemistry [6], 20 invariants were selected as significant predictors of physiochemical properties. The Symmetric division deg index is one of the discrete Adriatic indices which is a good predictor of total surface area for polychlorobiphenyls and some of the results on symmetric division deg index are also found in [3]. In [1], obtained an expression to introduce the symmetric division deg invariant of some derived graphs and its complements and also [7][] introduce a splice graph and its operations like edge subdivision, edge neighborhood subdivision, vertex neighborhood subdivision, vertex subdivision graphs,In this note we concentrated on inorganic clump graphs with a grith size of at most three. The girth of a graph is the length of the shortest cycle contained in a graph and is denoted by [g]. Since a tree has no cycles, we define its girth as infinity. It is shown that a complete graph with n-1 regular graphs shares many properties with a girth of size almost three.

2. Some clump graphs

From a chemical point of view, graphs with large number of edges may be considered as representations of inorganic clumps, called clump graphs. Bearing this in mind, we consider have the graphs obtained from the complete graphs K_s by removing some of its edges. In this section, we establish SDD invariant of following four types of clump graphs.

*Correspondence: s.p.murugarajan@gmail.com

Type I Let $e_i, i = 1, 2, ..., t, \quad 1 \leq t \leq s - 2$ be distinct edges of the complete graphs $K_s, \ s \geq 3$ all being incident to a single vertex. The graph $Ka_s(t)$ is obtained by deleting $e_i, i = 1, 2, ..., t$ from K_s. Note that $Ka_s(0) \cong K_s$.

Type II Let $e_i^{'}, i = 1, 2, ..., t, 1 \leq t \leq \left\lfloor \frac{s}{2} \right\rfloor$ be independent edges of the complete graph $Kb_s(t)$ is obtained by deleting $e_i^{'}, i = 1, 2, ..., t$ from K_s. Note that $Kb_s(0) \cong K_s$.

Type III Let V_t be a t element subset of the vertex set of $k_s, 2 \leq t \leq s-1, s \geq 3$. The graph $Kc_s(t)$ is obtained by deleting from K_s all the edges connecting pairs of vertices from V_t. Note that $Kc_s(0) \cong Kc_s(1) \cong K_s$.

Type IV Let $s \geq 3, 3 \geq t \geq s$. The graph $Kd_s(t)$ is obtained by deleting from K_s the edges belonging to a $t-$membered cycles.

Theorem 2.1. *For* $[g], s \geq 3$ *and* $1 \leq t \leq s-2,$, $SDD(Ka_s(t)) = t(t-1) + (s-t-1)(s-t-2) + \frac{2(s-1)^2 + t^2 - 2t(s-1)}{(s-1)} + t(s-t-1)\left[\frac{2s^2-6s+5}{(s-2)(s-1)}\right]$.

Proof: One can see that the graph $Ka_s(t)$ has s vertices and $\frac{s(s-1)}{2} - t$ edges. We can partition the edges set of $Ka_s(t)$ as follows;

$E_1 = \left\{a_1a_2 | \lambda_{Ka_s(t)}(a_1) = s-1-t, \lambda_{Ka_s(t)}(a_2) = s-1\right\}$.

$E_2 = \left\{a_1a_2 | \lambda_{Ka_s(t)}(a_1) = s-1, \lambda_{Ka_s(t)}(a_2) = s-2\right\}$.

$E_3 = \left\{a_1a_2 | \lambda_{Ka_s(t)}(a_1) = s-2, \lambda_{Ka_s(t)}(a_2) = s-1\right\}$.

$E_4 = \left\{a_1a_2 | \lambda_{Ka_s(t)}(a_1) = s-1, \lambda_{Ka_s(t)}(a_2) = s-1\right\}$.

Clearly $E(Ka_s(t)) = E_1 \cup E_2 \cup E_3 \cup E_4$ and $|E_1| = s-t-1$, $|E_2| = \frac{t(t-1)}{2}, |E_3| = t(s-t-1)$, $|E_4| = \frac{(s-t-1)(s-t-2)}{2}$. Hence

$$\begin{aligned}
SDD(Ka_s(t)) &= \sum_{i=1}^{4} \sum_{a_1a_2 \in E_i} \frac{\lambda_{Ka_s(t)}(a_1)^2 + \lambda_{Ka_s(t)}(a_2)^2}{\lambda_{Ka_s(t)}(a_1)\lambda_{Ka_s(t)}(a_2)} \\
&= (s-t-1)\Big[\frac{(s-t-1)^2 + (s-1)^2}{(s-t-1)(s-1)}\Big] + \frac{t(t-1)}{2}\Big[\frac{(s-2)^2 + (s-2)^2}{(s-2)(s-2)}\Big] \\
&+ t(s-t-1)\Big[\frac{(s-2)^2 + (s-1)^2}{(s-2)(s-1)}\Big] + \frac{(s-t-1)(s-t-2)}{2}\Big[\frac{(s-1)^2 + (s-1)^2}{(s-1)(s-1)}\Big] \\
&= \frac{(s-t-1)^2 + (s-1)^2}{(s-1)} + \frac{t(t-1)}{2}\Big[\frac{2(s-2)^2}{(s-2)^2}\Big] \\
&+ t(s-t-1)\Big[\frac{(s-2)^2 + (s-1)^2}{(s-2)(s-1)}\Big] + \frac{(s-t-1)(s-t-2)}{2}\Big[\frac{2(s-1)^2}{(s-1)^2}\Big] \\
&= t(t-1) + (s-t-1)(s-t-2) + \frac{2(s-1)^2 + t^2 - 2t(s-1)}{(s-1)} \\
&+ t(s-t-1)\Big[\frac{2s^2-6s+5}{(s-2)(s-1)}\Big].
\end{aligned}$$

Theorem 2.2. *For* $[g], s \geq 3$ *and* $1 \leq t \leq \left\lfloor \frac{t}{2} \right\rfloor$, $SDD(Kb_s(t)) = 2t(s-2t)\left[\frac{2s^2-6s+5}{(s-2)(s-1)}\right] + 2t(2t-1) + (s-$

$2t)(s-2t-1)-2t$.

Proof: One can easily check that the number of vertices and number of edges of $Kb_s(t)$ are respectively, s and $\frac{s(s-1)}{2}-t$. We can partition the edges set of $Kb_s(t)$ as follows;

$E_1=\left\{a_1a_2|\lambda_{Kb_s(t)}(a_1)=s-2,\lambda_{Kb_s(t)}(a_2)=s-1\right\}$.

$E_2=\left\{a_1a_2|\lambda_{Kb_s(t)}(a_1)=s-1,\lambda_{Kb_s(t)}(a_2)=s-1\right\}$.

$E_3=\left\{a_1a_2|\lambda_{Kb_s(t)}(a_1)=s-2,\lambda_{Kb_s(t)}(a_2)=s-2\right\}$.

We can observe that $|E_1|=2t(s-2t), |E_2|=\frac{(s-2t)(s-2t-1)}{2}, |E_3|=\left(\frac{2t(2t-1)}{2}\right)-t$ and $E(Kb_s(t))=E_1\cup E_2\cup E_3$. Thus

$$\begin{aligned}
SDD(Kb_s(t)) &= \sum_{i=1}^{3}\sum_{a_1a_2\in E_i}\frac{\lambda_{Kb_s(t)}(a_1)^2+\lambda_{Kb_s(t)}(a_2)^2}{\lambda_{Kb_s(t)}(a_1)\lambda_{Kb_s(t)}(a_2)}\\
&= 2t(s-2t)\Big[\frac{(s-2)^2+(s-1)^2}{(s-2)(s-1)}\Big]+\frac{(s-2t)(s-2t-1)}{2}\Big[\frac{(s-1)^2+(s-1)^2}{(s-1)(s-1)}\Big]\\
&+ \Big(\frac{2t(2t-1)}{2}-t\Big)\Big[\frac{(s-2)^2+(s-2)^2}{(s-2)(s-2)}\Big]\\
&= 2t(s-2t)\Big[\frac{(s-2)^2+(s-1)^2}{(s-2)(s-1)}\Big]+\frac{(s-2t)(s-2t-1)}{2}\Big[\frac{2(s-1)^2}{(s-1)^2}\Big]\\
&+ \Big(\frac{2t(2t-1)}{2}-t\Big)\Big[\frac{2(s-2)^2}{(s-2)^2}\Big]\\
&= 2t(s-2t)\Big[\frac{2s^2-6s+5}{(s-2)(s-1)}\Big]+2t(2t-1)+(s-2t)(s-2t-1)-2t.
\end{aligned}$$

Theorem 2.3. *For* $[g], s\geq 3$ *and* $2\leq t\leq s-1$, $SDD(Kc_s(t))=(s-t)(s-t-1)+t\Big[\frac{(s-t)^2+(s-1)^2}{(s-1)}\Big]$.

Proof: One can see that $|V((Kc_s(t)))|=s$ and $|E((Kc_s(t)))|=\frac{(s-t)(s-t-1)}{2}$. Moreover we can partition the edge set of the graph $Kc_s(t))$ as follows;

$E_1=\left\{a_1a_2|\lambda_{Kc_s(t)}(a_1)=s-t,\lambda_{Kc_s(t)}(a_2)=s-1\right\}$ and $|E_1|=(s-t)t$ and

$E_2=\left\{a_1a_2|\lambda_{Kc_s(t)}(a_1)=s-1,\lambda_{Kc_s(t)}(a_2)=s-1\right\}$ and $|E_2|=\frac{(s-t)(s-t-1)}{2}$. Hence

$$\begin{aligned}
SDD(Kc_s(t)) &= \sum_{i=1}^{2}\sum_{a_1a_2\in E_i}\frac{\lambda_{Kc_s(t)}(a_1)^2+\lambda_{Kc_s(t)}(a_2)^2}{\lambda_{Kc_s(t)}(a_1)\lambda_{Kc_s(t)}(a_2)}\\
&= (s-t)t\Big[\frac{(s-t)^2+(s-1)^2}{(s-t)(s-1)}\Big]+\frac{(s-t)(s-t-1)}{2}\Big[\frac{(s-1)^2+(s-1)^2}{(s-1)(s-1)}\Big]\\
&= t\Big[\frac{(s-t)^2+(s-1)^2}{(s-1)}\Big]+\frac{(s-t)(s-t-1)}{2}\Big[\frac{2(s-1)^2}{(s-1)^2}\Big]\\
&= (s-t)(s-t-1)+t\Big[\frac{(s-t)^2+(s-1)^2}{(s-1)}\Big].
\end{aligned}$$

Theorem 2.4. *For* $[g], s \geq 3$ *and* $2 \leq t \leq s-1$, $SDD(Kd_s(t)) = t(t-3)+(s-t)(s-t-1)+\Big(st-t^2\Big)\Big[\frac{2s^2-8s+10}{(s-3)(s-1)}\Big]$.

Proof: Note that $|V(Kd_s(t))| = s$ and $|E((Kd_s(t)))| = \frac{s(s-1)}{2} - t$. Form the structure of the graph $Kd_s(t)$ we have following edge partitions;

$E_1 = \big\{a_1a_2 | \lambda_{Kd_s(t)}(a_1) = s-3, \lambda_{Kd_s(t)}(a_2) = s-3\big\}$.

$E_2 = \big\{a_1a_2 | \lambda_{Kd_s(t)}(a_1) = s-3, \lambda_{Kd_s(t)}(a_2) = s-1\big\}$.

$E_3 = \big\{a_1a_2 | \lambda_{Kd_s(t)}(a_1) = s-1, \lambda_{Kd_s(t)}(a_2) = s-1\big\}$.

Moreover, $|E_1| = \frac{t(t-1)}{2} - t, |E_2| = t(s-t), |E_3| = \frac{(s-t)(s-t-1)}{2}$.

$$
\begin{aligned}
SDD(Kd_s(t)) &= \sum_{i=1}^{3} \sum_{a_1a_2 \in E_i} \frac{\lambda_{Kd_s(t)}(a_1)^2 + \lambda_{Kd_s(t)}(a_2)^2}{\lambda_{Kd_s(t)}(a_1)\lambda_{Kd_s(t)}(a_2)} \\
&= \Big(\frac{t(t-1)}{2} - t\Big)\Big[\frac{(s-3)^2 + (s-3)^2}{(s-3)(s-3)}\Big] + \Big(t(s-t)\Big)\Big[\frac{(s-3)^2 + (s-1)^2}{(s-3)(s-1)}\Big] \\
&\quad + \Big(\frac{(s-t)(s-t-1)}{2}\Big)\Big[\frac{(s-1)^2 + (s-1)^2}{(s-1)(s-1)}\Big] \\
&= \Big(\frac{t(t-1)}{2} - t\Big)\Big[\frac{2(s-3)^2}{(s-3)^2}\Big] + \Big(t(s-t)\Big)\Big[\frac{(s-3)^2 + (s-1)^2}{(s-3)(s-1)}\Big] \\
&\quad + \Big(\frac{(s-t)(s-t-1)}{2}\Big)\Big[\frac{2(s-1)^2}{(s-1)^2}\Big] \\
&= \Big(\frac{t(t-1)}{2} - t\Big)\Big(2\Big) + \Big(t(s-t)\Big)\Big[\frac{(s-3)^2 + (s-1)^2}{(s-3)(s-1)}\Big] \\
&\quad + \Big(\frac{(s-t)(s-t-1)}{2}\Big)\Big(2\Big) \\
&= t(t-1) - 2t + (st-t^2)\Big[\frac{(s-3)^2 + (s-1)^2}{(s-3)(s-1)}\Big] \\
&\quad + (s-t)(s-t-1) \\
&= t(t-3) + (s-t)(s-t-1) + \Big(st - t^2\Big)\Big[\frac{2s^2 - 8s + 10}{(s-3)(s-1)}\Big].
\end{aligned}
$$

3. Conclusion

In this note we have exhibited the existence of inorganic clump graphs and also evinced the exact values of SDD invariants of graphs with grith size atmost three.

References

[1] R. Aruldoss and P. Murugarajan, Derived Structures and Their Graph Invariants, South East Asian Journal of Mathematics and Mathematical Sciences, Vol No.17, (2021), pp13-22,2021

[2] A.T. Balaban, Highly discriminating distance based numerical descriptor, Chem. Phys. Lett., 89 (1982) 399-404.

[3] J. Devillers, A.T. Balaban, Topological Indices and Related Descriptors in QSAR and QSPR, Gordon and Breach, Amsterdam, 1999.

[4] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett., 17 (1972), 535-538.

[5] M. Karelson, Molecular Descriptors in QSAR/QSPR, Wiley-Interscience, New York, 2000.

[6] Milano Chemometrics & QSAR research group, molecular descriptors dataset, http://www.moleculardescriptors.eu/dataset/dataset.htm (accessed 18.04.14).

[7] P. Murugarajan and R. Aruldoss, Relation Between The S DD Invariant and Splice Graphs, Journal of Xian University of Architecture and Technology,Vol No XII,Issue XII,2020,pp113- 120.

[8] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc., 97 (1975) ,6609-6615.

[9] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.

[10] D. Vukicević., M. Gasperov, Bond aditive mdelling 1. Ariatic indices, Croat. Chem. Acta, 83 (2010), 243-260.

[11] H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc., 69 (1947) ,17-20.