Mathematical Biosciences and Engineering

http://www.aimspress.com/journal/mbe

MBE, 20(7): 11528–11544.
DOI: 10.3934/mbe.2023511
Received: 06 January 2023
Revised: 06 April 2023
Accepted: 11 April 2023
Published: 04 May 2023

Research article

Comparative study of five topological invariants of supramolecular chain of different complexes of N-salicylidene-L-valine

Xiujun Zhang[1], Umair Saleem[2], Muhammad Waheed[3], Muhammad Kamran Jamil[4,*] and Muhammad Zeeshan[3]

[1] School of Computer Science, Chengdu University, Chengdu, China

[2] Muslim Model Girls Higher Secondary School Zafarwal, Narowal, Pakistan

[3] Punjab School Education Department, Govt Higher Secondary School Nangal Sahdan Muridke, Sheikhupura, Pakistan

[4] Department of Mathematics, Riphah International University, Lahore, Pakistan

* **Correspondence:** Email: m.kamran.sms@gmail.com; Tel: +923464105447.

Abstract: L-valine is a crucial amino acid that has rising market demand and numerous uses. It can be used to make specific nutrients, animal feed additives, cosmetic ingredients, and other things in the medical and agricultural fields. N-salicylidene-L-valine (NsLv) is attracting a lot of attention due to its unusual structure and enhanced catalytic and cytotoxic activities. Topological index is a numerical value which is associated with the molecular structure. It is very helpful to predict physio-chemical properties and Quantitative structure-activity relationship and Quantitative structure-property relationship modeling. We study the supramolecular chain (Sc) in the dialkyl tin of complexes 2, 3 and 4 of NsLv to better understand this structure and its topological index-related characteristics. Additionally, we compare topological indices and analyze how these structures relate to one another using concrete examples.

Keywords: Sc in dialkyltin complex-2, 3 and 4; NsLv structure; topological indices

1. Introduction

The quantity of new drugs is growing daily due to the fast production of pharmaceuticals. Knowing the pharmacological, biological, and chemical features of these freshly manufactured medications is necessary to determine how effective they are against particular diseases. This is a laborious, time-consuming task that must be completed. When newly created medications fail to treat a particular condition, researchers work diligently to identify their shortcomings and increase their efficacy. This

requires well-established labs, reagents, and equipment. However, there is a lack of funding in developing nations to set up appropriate labs with all necessary reagents and equipment to assess the effectiveness of these medications. We have learned from the literature that the molecular structures of drugs and their chemical and pharmacologic effects are inextricably linked. If we compute measurements of drug molecular structures and find topological indices, pharmaceutical researchers can determine their medicinal characteristics. Deficiencies in their chemical experiments and structures, as well as their medicine, can be eliminated as a result. Therefore, the mathematical methods used to compute topological indices are especially useful for developing nations since they can forecast the pharmacological, biological, and chemical properties of medications without requiring laborious labor or laboratory studies.

In mathematics, the chemical structure of a drug can be represented as a graph, where the edges and vertices of the bonded atoms' chemical bonds are depicted. Consider a drug's chemical structure to be represented by the graph G, which has certain edges (chemical bonds between atoms) and vertices (bonded atoms). The topological index, which assigns a specific value to each molecular structure, converts the molecular composition of a given medicine into a numerical value that is a real-valued function. In the past 40 years, scientists have created numerous significant indices to identify the characteristics of molecules. These topological indices have established their value by finding significant uses in molecular graphs, engineering, and nanomaterials.

We examined the v-phenylenic nanotubes and nanotori fourth particle bond availability file in [1]. The benzenoid circumcoronene series Hk's third-connectivity and third-sum-connectivity indices are examined in [2]. The characteristics of the Sombor index for some nanostructures are discussed in [3], the topological indices of NEPS of graphs were computed in [4], the Zagreb connection index for drugs related to specific chemical structures was investigated in [5], and face index for silicon carbides was covered in [6]. Reference [7] discussed Zagreb connection indices of silicate, hexagonal, oxide, and honeycomb networks. Predicted values of first Zagreb connection index for random cyclooctatetraene chain, random polyphenyl chain and random chain network are reported in [8]. In [9] the author investigated the number of spanning trees, the Laplacian eigenvalues, and the Laplacian Estrada index of subdivided-line graphs. For more information, please refer to [10–18]. Twenty different amino acids are used to make proteins, and one of them is Lv, an essential amino acid for mammals. From Lv and salicylaldehyde, a chiral Schiff base carboxylate ligand known as NsLv is created, which has a remarkable capacity for coordination and many coordination modes toward metal ions. This ligand produces numerous metal complexes that are extensively used in research, particularly with regard to their characteristics and molecular structures [19–23]. These metal complexes are widely used as enantio-selective reaction catalysts, efficient reagents for DNA cleavage, and chiral fluorescent molecular sensors [24]. Organotin compounds, which are based on tin bonded to carbon, are organometallic compounds with a wide range of uses in materials science, organic synthesis, medicine and catalysis. Moreover, organotin compounds with carboxylate ligands have become compounds of great interest due to effective catalytic and cytotoxic activity along their various structures [25–27]. Organotin NsLv complexes exhibit significant biological and optical properties. They can be synthesized by combining sodium and potassium NsLv with either an oxide or a chloride [22,28,29]. Dialkyltin complexes of N-salicylidene-L-valine can be synthesized by heating and refluxing L-valine, salicylaldehyde, dialkyltin dichloride and DBU (1,8-diazabicyclo [5.4.0] undec-7-ene) in methanol for 4 hours in a round bottom flask. In the process, the remaining yellow residue is rinsed with water to dilute the Schiff base ligand,

DBU salt N-salicylidene-L-valinate, before it is evaporated by rotary evaporator in order to produce the pure product. For deeper information about the mechanism and synthesis of this structure, see [34].

Definitions

The reduced second Zagreb index [30] is defined as

$$RM_2(\Upsilon) = \sum_{uv \in E(\Upsilon)} \Big(d(u) - 1\Big)\Big(d(v) - 1\Big) \tag{1.1}$$

The reciprocal Randić index [31] is defined as

$$RR(\Upsilon) = \sum_{uv \in E(\Upsilon)} \sqrt{d(u)d(v)}. \tag{1.2}$$

The first and second Zagreb indices [32] are defined as

$$M_1(\Upsilon) = \sum_{v \in V(\Upsilon)} d(v)^2 = \sum_{uv \in E(\Upsilon)} \Big(d(u) + d(v)\Big) \tag{1.3}$$

$$M_2(\Upsilon) = \sum_{uv \in E(\Upsilon)} d(u)d(v). \tag{1.4}$$

The augmented Zagreb index [33] is defined as

$$AZI(\Upsilon) = \sum_{uv \in E(\Upsilon)} \Big(\frac{d(u)d(v)}{d(u) + d(v) - 2}\Big)^3 \tag{1.5}$$

2. Sc in dialkyltin complex-2,3,4 of NsLv

The four types of complexes found in the Sc of dialkyltin are NsLv complexes 2, 3, 4 and 5. Complexes $C_{2,\Psi}$, $C_{3,\Psi}$ and $C_{4,\Psi}$ will be covered in this section. The extended molecular structure unit graph shown in Figure 1 was created from the compound construction shown in Figure 2 [34]. Figure 7 shows the molecular structure's extended unit graph derived from the chemical structure shown in Figure 8, while Figure 4 displays the extended molecular structure unit graph created based on the chemical structure shown in Figure 5. The $C_{2,\Psi}$ have 1, 2, 3, 4 and 5 degree bonds. The $C_{3,\Psi}$ have 1, 2, 3 and 5 degree bonds. The $C_{4,\Psi}$ have 1, 2, 3 and 5 degree bonds. In addition, Tables 1, 3 and 5 display the edge type, degree of the end vertices-and frequency of the edge, all of which are extremely helpful to our computational work. The arrangement and size of $C_{2,\Psi}$- are $|V(C_{2,\Psi})| = 21\Psi$, $|E(C_{2,\Psi})| = 25\Psi - 2$, respectively. The order and size of $C_{3,\Psi}$- are $|V(C_{3,\Psi})| = 26\Psi$, $|E(C_{3,\Psi})| = 30\Psi - 1$, respectively. The order and size of $C_{4,\Psi}$- are $|V(C_{4,\Psi})| = 28\Psi$, $|E(C_{4,\Psi})| = 31\Psi - 1$, respectively.

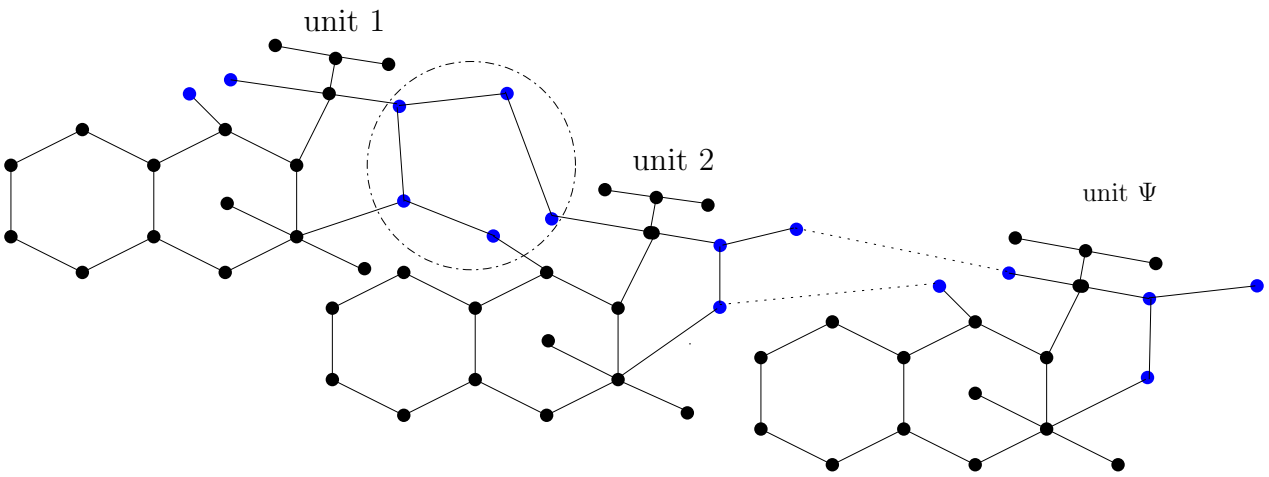

Figure 1. Sc in dialkyltin complex-2 of NsLv.

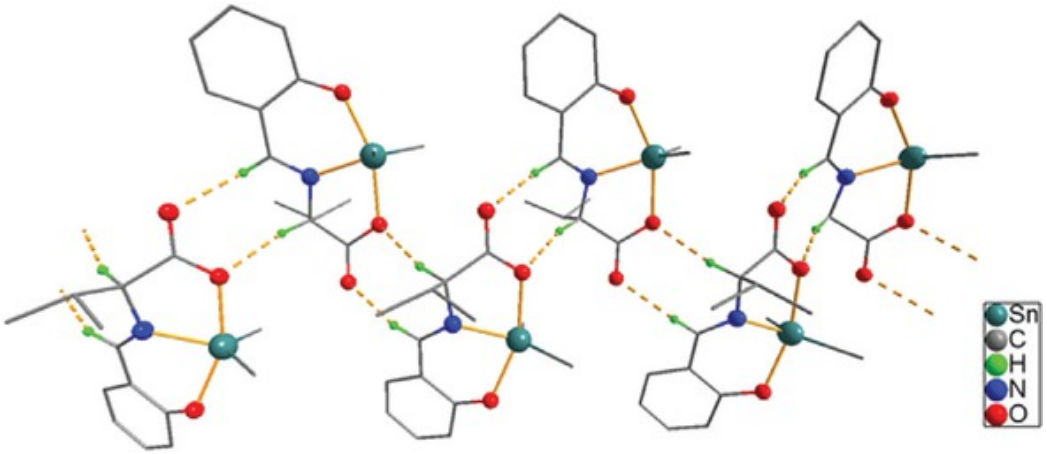

Figure 2. Sc in NsLv dialkyltin complex-2 chemical structure.

Table 1. The edge types with their end vertex degrees in $(C_{2,\Psi})$.

$(d(u), d(v))$	Frequency	$(d(u), d(v))$	Frequency
(2,2)	4Ψ-1	(3,3)	4Ψ-1
(2,3)	6Ψ-2	(1,5)	2Ψ
(1,3)	2Ψ+2	(2,5)	Ψ+1
(1,4)	1	(3,5)	2Ψ-1
(3,4)	3Ψ	(2,4)	Ψ-1

Theorem 1. *Let $C_{2,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-2, then the reduced second Zagreb index is,*

$$RM_2(C_{2,\Psi}) = 73\Psi - 16.$$

Proof. By referring to the definition of reduced second Zagreb index and Table 1,

$$\begin{aligned} RM_2(C_{2,\Psi}) =&(4\Psi - 1)(2 - 1)(2 - 1) + (6\Psi - 2)(2 - 1)(3 - 1) \\ &+ (2\Psi + 2)(1 - 1)(3 - 1) + (1)(1 - 1)(4 - 1) \\ &+ (3\Psi)(3 - 1)(4 - 1) + (4\Psi - 1)(3 - 1)(3 - 1) \\ &+ (2\Psi)(1 - 1)(5 - 1) + (\Psi + 1)(2 - 1)(5 - 1) \\ &+ (2\Psi - 1)(3 - 1)(5 - 1) + (\Psi - 1)(2 - 1)(4 - 1). \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$RM_2(C_{2,\Psi}) = 73\Psi - 16.$$

□

Theorem 2. *Let $C_{2,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-2, then the reciprocal Randić index is,*

$$RR(C_{2,\Psi}) = 66.7622\Psi - 7.97401.$$

Proof. By referring to the definition of reciprocal Randić index and Table 1,

$$\begin{aligned} RR(C_{2,\Psi}) =&(4\Psi - 1)\sqrt{2 \times 2} + (6\Psi - 2)\sqrt{2 \times 3} + (2\Psi + 2)\sqrt{1 \times 3} \\ &+ (1)\sqrt{1 \times 4} + (3\Psi)\sqrt{3 \times 4} + (4\Psi - 1)\sqrt{3 \times 3} \\ &+ (2\Psi)\sqrt{1 \times 5} + (\Psi + 1)\sqrt{2 \times 5} + (2\Psi - 1)\sqrt{3 \times 5} + (\Psi - 1)\sqrt{2 \times 4}. \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$RR(C_{2,\Psi}) = 66.7622\Psi - 7.97401.$$

□

Theorem 3. *Let $C_{2,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-2, then the first Zagreb index is,*

$$M_1(C_{2,\Psi}) = 140\Psi - 14.$$

Proof. By referring to the definition of first Zagreb index and Table 1,

$$\begin{aligned} M_1(C_{2,\Psi}) =&(4\Psi-1)(2+2)+(6\Psi-2)(2+3)+(2\Psi+2)(1+3)\\ &+(1)(1+4)+(3\Psi)(3+4)+(4\Psi-1)(3+3)+(2\Psi)(1+5)\\ &+(\Psi+1)(2+5)+(2\Psi-1)(3+5)+(\Psi-1)(2+4). \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$M_1(C_{2,\Psi}) = 140\Psi - 14.$$

□

Theorem 4. *Let $C_{2,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-2, then the second Zagreb index is,*

$$M_2(C_{2,\Psi}) = 188\Psi - 28.$$

Proof. By referring to the definition of second Zagreb index and Table 1,

$$\begin{aligned} M_2(C_{2,\Psi}) =&(4\Psi-1)(2\times 2)+(6\Psi-2)(2\times 3)+(2\Psi+2)(1\times 3)\\ &+(1)(1\times 4)+(3\Psi)(3\times 4)+(4\Psi-1)(3\times 3)+(2\Psi)(1\times 5)\\ &+(\Psi+1)(2\times 5)+(2\Psi-1)(3\times 5)+(\Psi-1)(2\times 4). \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$M_2(C_{2,\Psi}) = 188\Psi - 28.$$

□

Theorem 5. *Let $C_{2,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-2, then the augmented Zagreb index is,*

$$AZI(C_{2,\Psi}) = 224.94\Psi - 41.895.$$

Proof. By referring to the definition of augmented Zagreb index and Table 1,

$$\begin{aligned} AZI(C_{2,\Psi}) =&(4\Psi-1)\Big(\frac{2\times 2}{2+2-2}\Big)^3+(6\Psi-2)\Big(\frac{2\times 3}{2+3-2}\Big)^3+(2\Psi+2)\Big(\frac{1\times 3}{1+3-2}\Big)^3\\ &+(1)\Big(\frac{1\times 4}{1+4-2}\Big)^3+(3\Psi)\Big(\frac{3\times 4}{3+4-2}\Big)^3+(4\Psi-1)\Big(\frac{3\times 3}{3+3-2}\Big)^3\\ &+(2\Psi)\Big(\frac{1\times 5}{1+5-2}\Big)^3+(\Psi+1)\Big(\frac{2\times 5}{2+5-2}\Big)^3+(2\Psi-1)\Big(\frac{3\times 5}{3+5-2}\Big)^3\\ &+(\Psi-1)\Big(\frac{2\times 4}{2+4-2}\Big)^3. \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$AZI(C_{2,\Psi}) = 224.94\Psi - 41.895.$$

□

Table 2. Comparison of topological values in ($C_{2,\Psi}$).

Ψ	RM_2	RR	M_1	M_2	AZI
1	57	58.78819	126	160	183.045
2	130	125.55039	266	348	407.985
3	203	192.31259	406	536	632.925
4	276	259.07479	546	724	857.865
5	349	325.83699	686	912	1082.805
6	422	392.59919	826	1100	1307.745
7	495	459.36139	966	1288	1532.685

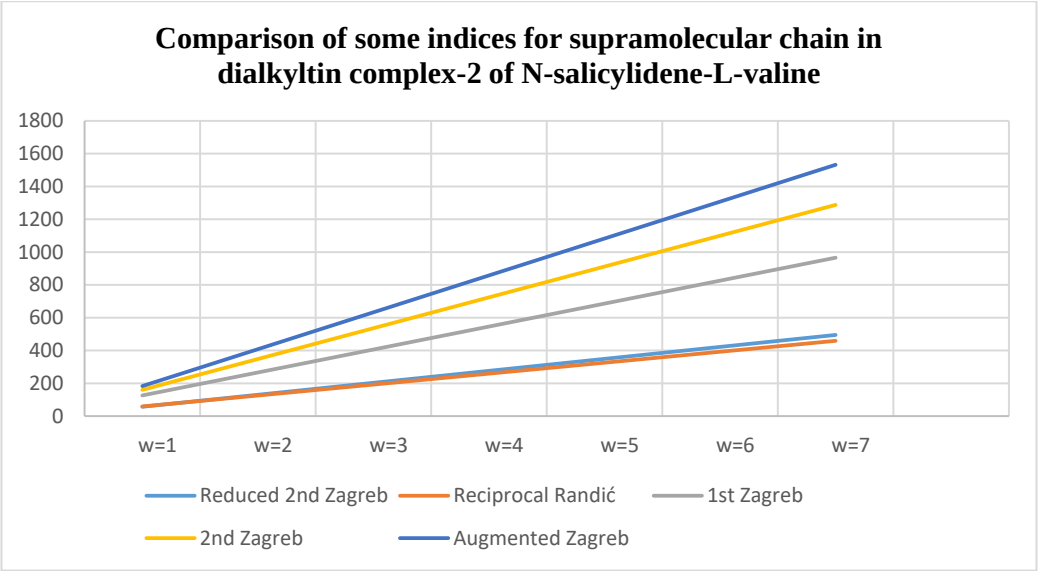

Figure 3. Graphical comparison of some indices for Sc in dialkyltin complex-2 of NsLv.

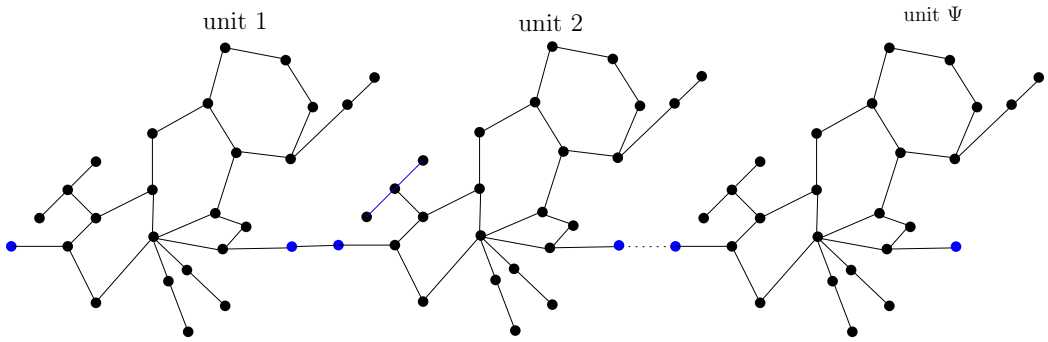

Figure 4. Sc in dialkyltin complex-3 of NsLv.

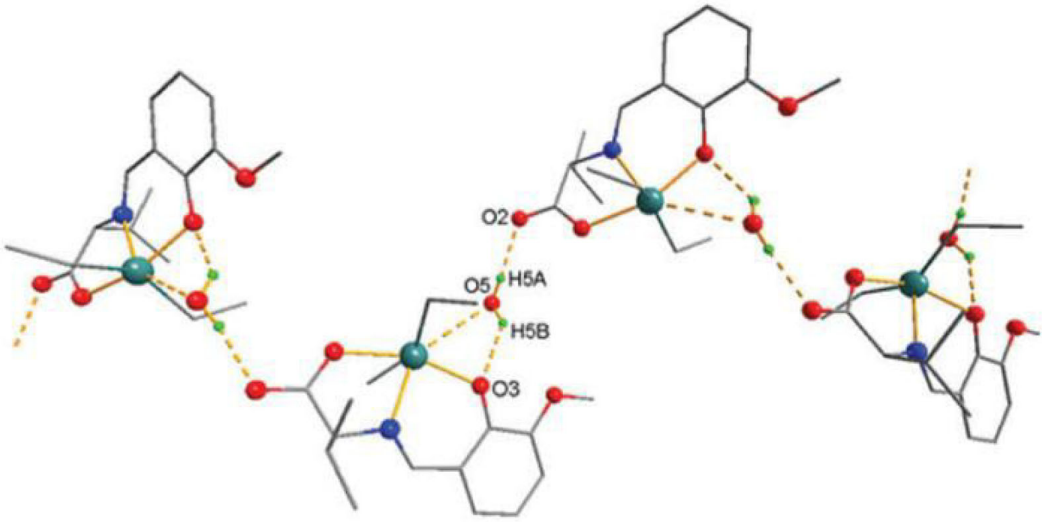

Figure 5. Chemical structure Sc in dialkyltin complex-3 of NsLv.

Table 3. The edge types with their end vertex degrees in $(C_{3,\Psi})$.

$(d(u), d(v))$	Frequency	$(d(u), d(v))$	Frequency
(1,2)	3Ψ	(1,3)	2Ψ+2
(2,3)	10Ψ-2	(2,6)	3Ψ
(2,2)	3Ψ-1	(3,6)	3Ψ
(3,3)	6Ψ		

Theorem 6. *Let $C_{3,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-3, then the reduced second Zagreb index is,*

$$RM_2(C_{3,\Psi}) = 92\Psi - 5.$$

Proof. By using the definition of reduced second Zagreb index and Table 3,

$$\begin{aligned} RM_2(C_{3,\Psi}) =& (3\Psi)(1-1)(2-1) + (10\Psi-2)(2-1)(3-1) \\ &+ (3\Psi-1)(2-1)(2-1) + (6\Psi)(3-1)(3-1) \\ &+ (2\Psi+2)(1-1)(3-1) + (3\Psi)(2-1)(6-1) \\ &+ (3\Psi)(3-1)(6-1). \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$RM_2(C_{3,\Psi}) = 92\Psi - 5.$$

□

Theorem 7. *Let $C_{3,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-3, then the reciprocal Randić index is*

$$RR(C_{3,\Psi}) = 79.313\Psi - 3.434.$$

Proof. By referring to the definition of reciprocal Randić index and Table 3,

$$\begin{aligned} RR(C_{3,\Psi}) =&(3\Psi)\sqrt{1\times 2}+(10\Psi-2)\sqrt{2\times 3}+(3\Psi-1)\sqrt{2\times 2}\\ &+(6\Psi)\sqrt{3\times 3}+(2\Psi+2)\sqrt{1\times 3}+(3\Psi)\sqrt{2\times 6}\\ &+(3\Psi)\sqrt{3\times 6}. \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$RR(C_{3,\Psi}) = 79.313\Psi - 3.434.$$

□

Theorem 8. *Let $C_{3,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-3, then the first Zagreb index is*

$$M_1(C_{3,\Psi}) = 166\Psi - 6.$$

Proof. By referring to the definition of first Zagreb index and Table 3,

$$\begin{aligned} M_1(C_{3,\Psi}) =&(3\Psi)(1+2)+(10\Psi-2)(2+3)+(3\Psi-1)(2+2)\\ &+(6\Psi)(3+3)+(2\Psi+2)(1+3)+(3\Psi)(2+6)\\ &+(3\Psi)(3+6). \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$M_1(C_{3,\Psi}) = 166\Psi - 6.$$

□

Theorem 9. *Let $C_{3,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-3, then the second Zagreb index is*

$$M_2(C_{3,\Psi}) = 228\Psi - 10.$$

Proof. By referring to the definition of second Zagreb index and Table 3,

$$\begin{aligned} M_2(C_{3,\Psi}) =&(3\Psi)(1\times 2)+(10\Psi-2)(2\times 3)+(3\Psi-1)(2\times 2)\\ &+(6\Psi)(3\times 3)+(2\Psi+2)(1\times 3)+(3\Psi)(2\times 6)\\ &+(3\Psi)(3\times 6). \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$M_2(C_{3,\Psi}) = 228\Psi - 10.$$

□

Theorem 10. *Let $C_{3,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-3, then the augmented Zagreb index is*

$$AZI(C_{3,\Psi}) = 278.07\Psi - 17.25.$$

Proof. By referring to the definition of augmented Zagreb index and Table 3,

$$\begin{aligned} AZI(C_{3,\Psi}) =&(3\Psi)\Big(\frac{1\times 2}{1+2-2}\Big)^3 + (10\Psi-2)\Big(\frac{2\times 3}{2+3-2}\Big)^3 + (3\Psi-1)\Big(\frac{2\times 2}{2+2-2}\Big)^3 \\ &+ (6\Psi)\Big(\frac{3\times 3}{3+3-2}\Big)^3 + (2\Psi+2)\Big(\frac{1\times 3}{1+3-2}\Big)^3 + (3\Psi)\Big(\frac{2\times 6}{2+6-2}\Big)^3 \\ &+ (3\Psi)\Big(\frac{3\times 6}{3+6-2}\Big)^3. \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$AZI(C_{3,\Psi}) = 278.07\Psi - 17.25.$$

□

Table 4. Comparison of topological values in $(C_{3,\Psi})$.

Ψ	RM_2	RR	M_1	M_2	AZI
1	87	75.879	160	218	260.82
2	179	155.192	326	446	538.89
3	271	234.505	492	674	816.96
4	363	313.818	658	902	1095.03
5	455	393.131	824	1130	1373.1
6	547	472.444	990	1358	1651.17
7	639	551.757	1156	1586	1929.24

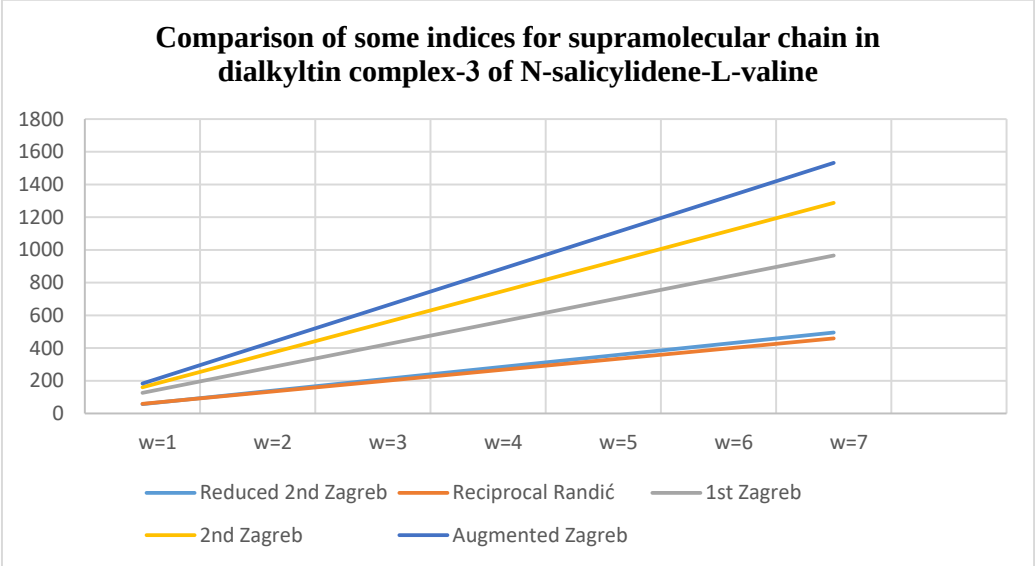

Figure 6. Graphical comparison of some indices for Sc in dialkyltin complex-3 of NsLv.

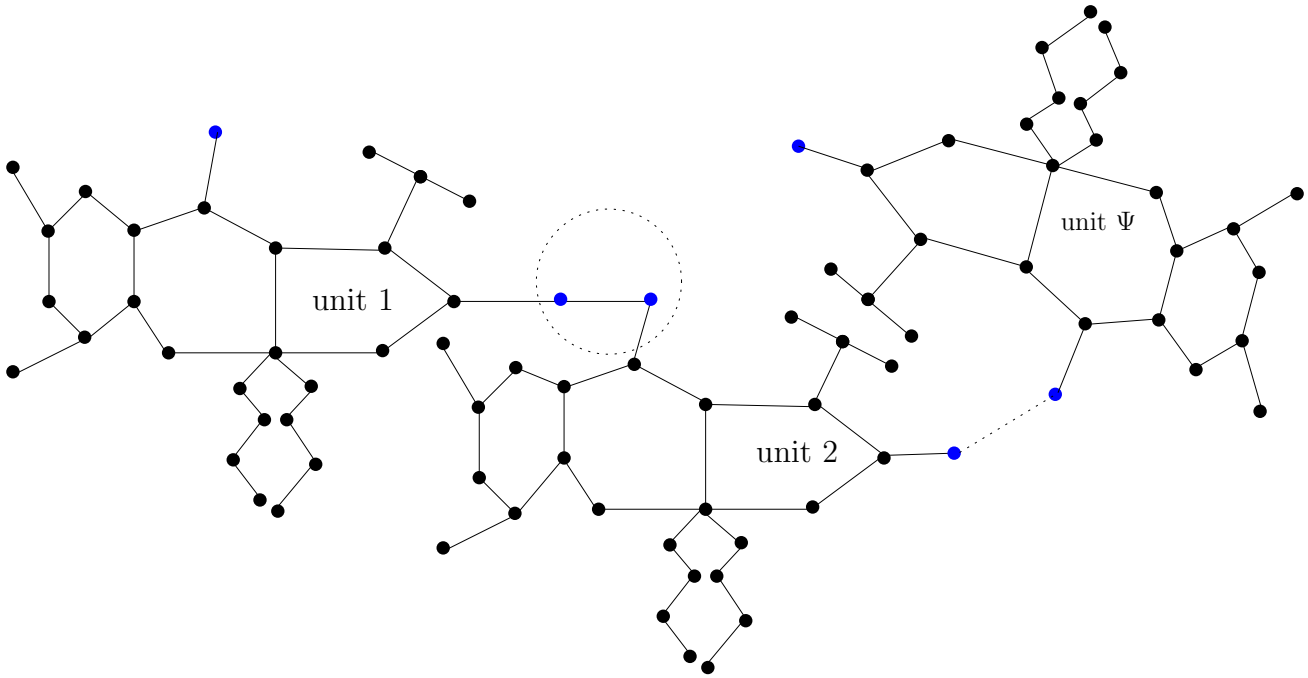

Figure 7. Sc in dialkyltin complex-4 of NsLv.

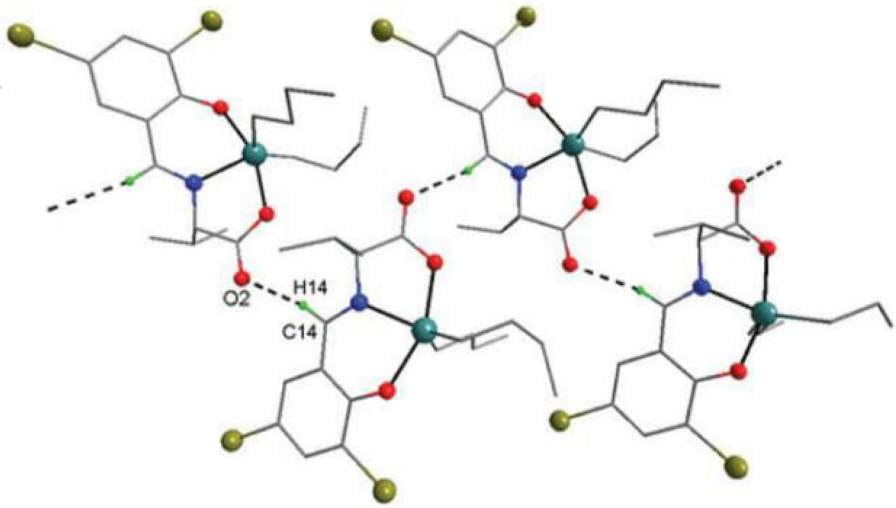

Figure 8. Chemical structure Sc in dialkyltin complex-4 of NsLv.

Table 5. The edge types with their end vertex degrees in $(C_{4,\Psi})$.

$(d(u), d(v))$	Frequency	$(d(u), d(v))$	Frequency
(1,3)	4Ψ+2	(2,2)	5Ψ-1
(2,3)	8Ψ-2	(2,5)	4Ψ
(3,3)	7Ψ	(3,5)	Ψ
(1,2)	2Ψ		

Theorem 11. *Let $C_{4,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-4, then the reduced second Zagreb index is*

$$RM_2(C_{4,\Psi}) = 73\Psi - 5.$$

Proof. By referring to the definition of reduced second Zagreb index and Table 5,

$$\begin{aligned} RM_2(C_{4,\Psi}) =& (4\Psi + 2)(1-1)(3-1) + (8\Psi - 2)(2-1)(3-1) \\ &+ (7\Psi)(3-1)(3-1) + (2\Psi)(1-1)(2-1) \\ &+ (5\Psi - 1)(2-1)(2-1) + (4\Psi)(2-1)(5-1) \\ &+ (\Psi)(3-1)(5-1). \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$RM_2(C_{4,\Psi}) = 73\Psi - 5.$$

□

Theorem 12. *Let $C_{4,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-4, then the reciprocal Randić index is*

$$RR(C_{4,\Psi}) = 76.8746\Psi - 3.43488.$$

Proof. By referring to the definition of reciprocal Randić index and Table 5,

$$\begin{aligned} RR(C_{4,\Psi}) =& (4\Psi + 2)\sqrt{1\times 3} + (8\Psi - 2)\sqrt{2\times 3} + (7\Psi)\sqrt{3\times 3} \\ &+ (2\Psi)\sqrt{1\times 2} + (5\Psi - 1)\sqrt{2\times 2} + (4\Psi)\sqrt{2\times 5} \\ &+ (\Psi)\sqrt{3\times 5}. \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$RR(C_{4,\Psi}) = 76.8746\Psi - 3.43488.$$

□

Theorem 13. *Let $C_{4,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-4, then the first Zagreb index is*

$$M_1(C_{4,\Psi}) = 160\Psi - 6.$$

Proof. By referring to the definition of first Zagreb index and Table 5,

$$\begin{aligned} M_1(C_{4,\Psi}) =&(4\Psi + 2)(1 + 3) + (8\Psi - 2)(2 + 3) + (7\Psi)(3 + 3) \\ &+ (2\Psi)(1 + 2) + (5\Psi - 1)(2 + 2) + (4\Psi)(2 + 5) \\ &+ (\Psi)(3 + 5). \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$M_1(C_{4,\Psi}) = 160\Psi - 6.$$

□

Theorem 14. *Let $C_{4,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-4, then the second Zagreb index is*

$$M_2(C_{4,\Psi}) = 202\Psi - 10.$$

Proof. By referring to the definition of second Zagreb index and Table 5,

$$\begin{aligned} M_2(C_{4,\Psi}) =&(4\Psi + 2)(1 \times 3) + (8\Psi - 2)(2 \times 3) + (7\Psi)(3 \times 3) + (2\Psi)(1 \times 2) \\ &+ (5\Psi - 1)(2 \times 2) + (4\Psi)(2 \times 5) + (\Psi)(3 \times 5). \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$M_2(C_{4,\Psi}) = 202\Psi - 10.$$

□

Theorem 15. *Let $C_{4,\Psi}$, with $\Psi \geq 1$ is a Sc graph in NsLv dialkyltin complex-4, then the augmented Zagreb index is*

$$AZI(C_{4,\Psi}) = 260.856\Psi - 17.25.$$

Proof. By referring to the definition of augmented Zagreb index and Table 5,

$$\begin{aligned} AZI(C_{4,\Psi}) =&(4\Psi + 2)\Big(\frac{1 \times 3}{1 + 3 - 2}\Big)^3 + (8\Psi - 2)\Big(\frac{2 \times 3}{2 + 3 - 2}\Big)^3 + (7\Psi)\Big(\frac{3 \times 3}{3 + 3 - 2}\Big)^3 \\ &+ (2\Psi)\Big(\frac{1 \times 2}{1 + 2 - 2}\Big)^3 + (5\Psi - 1)\Big(\frac{2 \times 2}{2 + 2 - 2}\Big)^3 + (4\Psi)\Big(\frac{2 \times 5}{2 + 5 - 2}\Big)^3 \\ &+ (\Psi)\Big(\frac{3 \times 5}{3 + 5 - 2}\Big)^3. \end{aligned}$$

After simplifying the preceding statement, we get the following result:

$$AZI(C_{4,\Psi}) = 260.856\Psi - 17.25.$$

□

Table 6. Comparison of topological values in ($C_{4,\Psi}$).

Ψ	RM_2	RR	M_1	M_2	AZI
1	68	73.43972	154	192	243.606
2	141	150.31432	314	394	504.462
3	214	227.18892	474	596	765.318
4	287	304.06352	634	798	1026.174
5	360	380.93812	794	1000	1287.03
6	433	457.81272	954	1202	1431.54
7	506	534.68732	1114	1404	1808.742

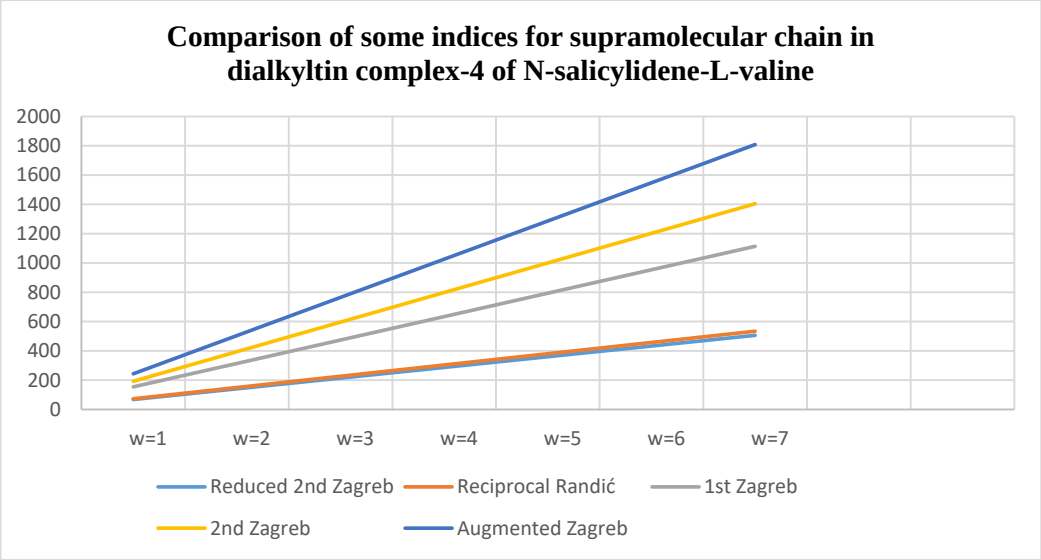

Figure 9. Graphical comparison of some indices for Sc in dialkyltin complex-4 of NsLv.

3. Discussion

For the purpose of examining topological indices, chemical structures and their designed networks of vertices and edges are thought to be useful tools. You can observe how a particular structure and graph behave using topological indices, which offer numerical values. The five degree-based topological indices of our table-based structure that are the subject of the report are examined. Corresponding graphs were created using parameter values ranging from 1 to 7 for each of the five topological indices. Figure 3 plots five degree-based topological indices for the structure of the Sc in dialkyltin complex-2 of NsLv ($C_{2,\Psi}$) based on the information in Table 2. The plots grow in size linearly. The reciprocal Randić index and the reduced second Zagreb index are close to each other, but overall the reciprocal Randić index moves sharply in size among the others in ($C_{2,\Psi}$). The structure of the Sc in dialkyltin complex-3 of NsLv ($C_{3,\Psi}$) is depicted in Figure 6 as a plot of five degree based topological indices derived from Table 4 data. The plots expand in size in a linear fashion. The reciprocal Randić index

and the second-reduced Zagreb index are close to one another, but generally the reciprocal Randić index moves sharply in size among the others in $(C_{3,\Psi})$. Because of the structure of the Sc in dialkyltin complex-4 of NsLv $(C_{4,\Psi})$ data from Table 6 are used to generate a plot of five degree-based topological indices in Figure 9. The plots enlarge linearly. The reciprocal Randić index and the reduced second Zagreb index are close together, however, in comparison to the others, the scaled-down second Zagreb index moves dramatically in size. $(C_{4,\Psi})$. It makes sense to assume that when examining our chosen structures $(C_{2,\Psi})$ and $(C_{3,\Psi})$, the reciprocal Randić index is preferable to the others, but when examining $(C_{4,\Psi})$ the reduced second Zagreb index is more appropriate for study than the others.

4. Conclusions

The chemical structure known as a Sc in the dialkyltin complexes-2, 3 and 4 of NsLv was examined in this study using computational methods. We investigated some relevant topological descriptors, such as the reduced second Zagreb index, the reciprocal Randić index, the first and second Zagreb index- and the augmented Zagreb index, to examine the behavior of our selected structures. As future work, many other degree and distance based entropies such as Sombor based, eccentricity based and Wiener based entropies can be computed for these structures.

Conflict of interest

The authors declare there is no conflict of interest.

References

1. M. R. Farahani, Computing fourth atom-bond connectivity indexof v-phenylenic nanotubes and nanotori, *Acta Chim. Slov.*, **60** (2013), 429–432.
2. M. R. Farahani, Third-Connectivity and third-sum-connectivity indices of circumcoronene series of Benzenoid H_k, *Acta Chim. Slov.*, **60** (2013), 198–202.
3. A. Alsinai, B. Basavanagoud, M. Sayyed, M. R. Farahani, Sombor index of some nanostructures, *J. Prime Res. Math.*, **17** (2021), 123–133.
4. M. Imran, S. Akhter, M. K. Jamil, Computation of topological indices of NEPS of graphs, *Complexity*, (2021). https://doi.org/10.1155/2021/9911226
5. M. I. Qureshi, A. Fahad, M. K. Jamil, S. Ahmad, Zagreb Connection index of drugs related chemical structures, *Biointerface Res. Appl. Chem.*, **4** (2021), 11920–11930. https://doi.org/10.33263/BRIAC114.1192011930
6. X. Zhang, A. Raza, A. Fahad, M. K. Jamil, M. A. Chaudhry, Z. Iqbal, On face index of silicon carbides, *Discrete Dyn. Nat. Soc.*, (2020). https://doi.org/10.1155/2020/6048438
7. A. Fahad, A. Aslam, M. I. Qureshi, M. K. Jamil, A. Jaleel, Zagreb connection indices of some classes of networks, *Biointerface Res. Appl. Chem.*, **3** (2021), 10074–10081.

8. Z. Raza, S. Akhter, Y. Shang, Expected value of first Zagreb connection index in random cyclooctatetraene chain, random polyphenyls chain, and random chain network, *Front. Chem.*, **10** (2023). https://doi.org/10.3389/fchem.2022.1067874
9. Y. Shang, On the number of spanning trees, the Laplacian eigenvalues, and the Laplacian Estrada index of subdivided-line graphs, *Open Math.*, **14** (2016), 641–648.
10. X. Zhang, H. M. Awais, M. Javaid, M. K. Siddiqui, Multiplicative Zagreb indices of molecular graphs, *J. Chem.*, **2019** (2019). https://doi.org/10.1155/2019/5294198
11. X. Zhang , H. Jiang, J. B. Liu, Z. Shao, The cartesian product and join graphs on edge-version atom-bond connectivity and geometric aritheoetic indices, *Molecules*, **23** (2018), 1731–1746. https://doi.org/10.3390/molecules23071731
12. X. Zhang, A. Rauf, M. Ishtiaq, M. K. Siddiqui, M. H. Muhammad, On degree based topological properties of two carbon nanotubes, *Polycyclic Aromat. Compd.*, **42** (2020), 866–884. https://doi.org/10.1080/10406638.2020.1753221
13. J. B. Liu, Q. Xie, J. J. Gu, Statistical analyses of a class of random pentagonal chain networks with respect to several topological properties, *J. Funct. Spaces*, (2023). https://doi.org/10.1155/2023/6675966
14. X. Zhang, A. Raza, A. Fahad, M. K. Jamil, M. A. Chaudhry, Z. Iqbal, On face index of silicon carbides, *Discrete Dyn. Nat. Soc.*, **2020** (2020). https://doi.org/10.1155/2020/6048438
15. F. Deng, X. Zhang, M. Alaeiyan, A. Mehboob, M. R. Farahani, Topological Indices of the Pent-Heptagonal Nanosheets VC_5C_7 and HC_5C_7, *Adv. Mater. Sci. Eng.*, (2019).
16. J. B. Liu, Y. Bao, W. T. Zheng, Analyses of some structural properties on a class of hierarchical scale-free networks, *Fractals*, **30** (2022). https://doi.org/10.1142/S0218348X22501365
17. J. B. Liu, C. Wang, S. Wang, B. Wei, Zagreb indices and multiplicative zagreb indices of eulerian graphs, *Bull. Malays. Math. Sci. Soc.*, **42** (2019), 67–78. https://doi.org/10.1007/s40840-017-0463-2
18. X. Zhang, Z. Zhang, N. Chidambaram, On degree and distance-based topological indices of certain interconnection networks, *Eur. Phys. J. Plus*, **137** (2022). https://doi.org/10.1140/epjp/s13360-022-03010-0
19. Y. N. Belokon, V. I. Maleev, D. A. Kataev, T. F. Saveleva, T. V. Skrupskaya, Y. V. Nelyubina, et al., Chiral ion pairs in catalysis: lithium salts of chiral metallocomplex anions as catalysts for asymmetric C–C bond formation, *Tetrahedron: Asymmetry*, **20** (2009), 1746–1752. https://doi.org/10.1016/j.tetasy.2009.06.006
20. C. T. Chen, S. Bettigeri, S. S. Weng, V. D. Pawar, Y. H. Lin, C. Y. Liu, et al., Asymmetric aerobic oxidation of alpha-hydroxy acid derivatives by c_4-symmetric, vanadate-centered, tetrakis Vanadyl (V) clusters derived from N-salicylidene-alpha-aminocarboxylates, *J. Org. Chem.*, **72** (2007), 8175–8185. https://doi.org/10.1021/jo070575f
21. C. T. Chen, J. S. Lin, J. H. Kuo, S. S. Weng, T. S. Cuo, Y. W. Lin, et al., Site-Selective DNA photocleavage involving unusual photoinitiated tautomerization of chiral tridentate Vanadyl (V) complexes derived from N-Salicylidene alpha-amino acids, *Org. Lett.*, **6** (2004), 4471–4474. https://doi.org/10.1021/ol048156h

22. A. Ucar, M. Findik, H. Bingol, E. Guler, E. Ozcan, Organometallic chiral schiff base for enantioSelective fluorescent recognition of methionine, *Chem. Papers*, **71** (2017), 1855–1862.

23. J. Yu, H. J. Jiang, Y. Zhou, S. W. Luo, L. Z. Gong, Sodium salts of anionic chiral cobalt (III) complexes as catalysts of the enantioselective povarov reaction, *Angew. Chem.*, **54** (2015), 11209–11213. https://doi.org/10.1002/anie.201504790

24. A. G. Davies, M. Gielen, K. H. Pannell, E. R. T. Tiekink, Tin chemistry: Fundamentals, frontiers, and applications, *J. Am. Chem. Soc.*, **15** (2008), 752. https://doi.org/10.1007/978-3-031-02484-9_3

25. F. Arjmand, S. Parveen, S. Tabassum, C. Pettinari, Organotin antitumor compounds: Their present status in drug development and future perspectives, *Inorg. Chim. Acta*, **423** (2014), 26–37. https://doi.org/10.1016/j.ica.2014.07.066

26. C. N. Banti, S. K. Hadjikakou, T. Sismanoglu, N. Hadjiliadis, Anti-proliferative and antitumor activity of organotin(IV) compounds. An overview of the last decade and future perspectives, *J. Inorg. Biochem.*, **194** (2019), 114–152. https://doi.org/10.1016/j.jinorgbio.2019.02.003

27. L. J. Tian, L. X. Chen, W. G. An, X. C. Liu, Diorganotin complexes of N-[4-(Diethylamino)Salicylidene]-L-Tryptophane: Syntheses, structures and properties, *Chin. J. Struct. Chem.*, **38** (2019), 1977–1985.

28. H. I. Beltran, L. S. Z. Rivera, T. Mancilla, R. Santillan, N. Farfan, One-Step preparation, structural assignment, and X-ray study of 2,2-di-n-butyl- and 2,2-diphenyl-6-aza-1,3-dioxa-2-stannabenzocyclononen-4-ones derived from amino acids, *Chemistry*, **9** (2003), 2291–2306. https://doi.org/10.1002/chem.200204260

29. Y. Yao, M. Yang, X. Zheng, L. Tian, Synthesis, characterization, and cytotoxic activity of triphenyltin complexes of N-(5-Bromosalicylidene)-α-amino acids, *Main Group Met. Chem.*, **40** (2017), 93–99.

30. A. Abdussakir, Some topological indices of subgroup graph of symmetric group, *Math. Stat.*, **7** (2019), 98–105. https://doi.org/10.13189/MS.2019.070402

31. F. C. G. Manso, H. S. Júnior, R. E. Bruns, A. F. Rubira, E. C. Muniz, Development of a new topological index for the prediction of normal boiling point temperatures of hydrocarbons: The Fi index, *J. Mol. Liq.*, **165** (2012), 125–132. https://doi.org/10.1016/j.molliq.2011.10.019

32. M. Ghorbani, A. M. Hosseinzadeh, A new version of Zagreb indices, *Filomat*, **26** (2012), 93–100. https://doi.org/10.2298/FIL1201093G

33. B. Furtula, A. Graovac, D. Vukičević, Augmented Zagreb index, *J. Math. Chem.*, **48** (2010), 370–380. https://doi.org/10.1007/s10910-010-9677-3

34. L. Tian, R. Wang, J. Zhang, F. Zhong, Y. Qiu, Synthesis and structural characterization of dialkyltin complexex of N-Salicylidene-L-Valine, *Main Group Met.Chem.*, **43** (2020), 138–146. https://doi.org/10.1515/mgmc-2020-0017

AIMS Press