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Editorial: Topological investigations of chemical networks

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Abstract: The topic of computing the topological indices (TIs) being a graph-theoretic modeling of the networks or discrete structures has become an important area of research nowadays because of its immense applications in various branches of the applied sciences. TIs have played a vital role in mathematical chemistry since the pioneering work of famous chemist Harry Wiener in 1947. However, in recent years, their capability and popularity has increased significantly because of the findings of the different physical and chemical investigations in the various chemical networks and the structures arising from the drug designs. In additions, TIs are also frequently used to study the quantitative structure property relationships (QSPRs) and quantitative structure activity relationships (QSARs) models which correlate the chemical structures with their physio-chemical properties and biological activities in a dataset of chemicals. These models are very important and useful for the research community working in the wider area of cheminformatics which is an interdisciplinary field combining mathematics, chemistry, and information science. The aim of this editorial is to arrange new methods, techniques, models, and algorithms to study the various theoretical and computational aspects of the different types of these topological indices for the various molecular structures.

Keywords: chemical structures, topological indices, graph-theoretic techniques

1 Introduction and preliminaries

For a finite nonempty set V, a graph G(V; E) being a pair of two sets V and $E \subset V \times V$ can be visualized by representing the elements of V by nodes or vertices and joining an unordered pair of vertices (u; v) by a bond or edge if and only if $(u; v) \in E(G)$ (Harary, 1969). The cardinality of the vertex set V is called order and cardinality of the edge-set E is known by the size of the graph G(V; E). It is very important to report here that first of all the term of graph is introduced by Sylvester (1874). Moreover, two graphs $G_1(V_1; E_1)$ and $G_2(V_2; E_2)$ are isomorphic if there exists a bijective function f from V_1 to V_2 that preserves the adjacency i.e for any pair of vertices u, v of G_1 if $(u; v) \in E_1$ then $(f(u); f(v)) \in E_2$ and vice versa. The degree of a vertex of a graph is number of incident edges on it. A walk is an alternating sequence of vertices and edges in which any two consecutive vertices are adjacent and a walk is called by path if no vertex is repeated. The distance between two vertices of a graph is length (number of edges) of the shortest path between them. For more details, see Harary (1969).

The molecules being the smallest possible units play a role of building blocks by different ways of chemically bonding for a compound or chemical. In this study, a chemical formula presents the actual number of atoms for each molecule of the chemical and a structural formula provide a geometrically presentation in which the atoms of the molecules are linked or chemically bonded. Two or more compounds (chemicals) are said to make a class of structural isomer if they have same chemical but different structural formulas. For example, two compounds butanol and methyl propyl ether are structural isomer because they have the same molecular formula $C_{\nu}H_{10}O$ and different structural formulas $H_3C-(CH_2)_3-OH$ and $H_3C-(CH_2)_3-O-OH_2$, respectively. Moreover, molecular graphs can be distinguished in a class of chemical graphs under the condition of structural isomers. In another way, a chemical graph is said to be a molecular graph if the degree of each vertex is less than four. For more details, we refer to Gutman and Polansky (1986).

Chemical graph theory is a branch of mathematical chemistry that studies the physical and chemical

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properties (boiling points, freezing point, melting points, molar refraction, acentric factor, motor octane number, octanol-water partition coefficient, surface tension and density, heat of formation and solubility) of the chemical graphs with the help of the mathematical models which are prepared by the graph-theoretic techniques of the subject of graph theory.

In addition, an interesting emerging subfield called cheminformatics deals with a chemical phenomenon known as quantitative structure activity and structureproperty relationships of chemical compounds. The methods of cheminformatics are also used for the prediction of properties relevant to the drug discovery and optimization process. For example, knowledge discovery can be used for the identification of lead compounds in pharmaceutical data matching. As this era is dedicated to the advancements in chemical sciences such as drug discovery, bond formation in chemical compounds and development of diagnosis kits for different diseases and biological processes. All these developments require tools that will make possible these advancements to propel the way they are propelling.

An emerging tool, used in the study of these phenomena, is a topological index which remains constant for all chemical structures up to their isomorphisms. The branch of graph theory in which a chemical compounds picturesque image namely, molecular graph is used to analyse the compounds different physio-chemical properties with numeric identifiers namely topological indices (TI). There are various types of topological indices such as degree, distance and polynomial based but degree-based are more studied than others, see the latest survey of Gutman (2013).

Wiener is regarded as the founder of TI. While finding the boiling point of paraffin during a lab activity (Wiener, 1947). He called it path number. Latter the same was proclaimed as Wiener index. Afterwards, this area has flourished with a large number of new kind of TI and many researchers have developed in terms of connectivity, eccentricity, degree, and distance based aspects of a molecular graph which atoms are regarded as nodes/vertices and bonds between them are shown by edges. A bunch of topological descriptors based on aforesaid properties of graphs are classic Zagrab indices developed by Gutman and Trinajstic (1972) widely known as first and second Zagreb indices. Furtula and Gutman (2015) based on degree of a chemical graph defined 3rd Zagreb indices. Afterwards, Randić used indices as the branching indices (Randic, 1975). Recently, Wasson et al. (2008) gave the idea of linker competition within a metalorganic framework (MON) for topological insights.

In this note, we are concerned with new developments on networks and chemical structures namely metal organic

framework (MOF), dendrimers, carbon nano-sheets, and planar octahedral networks under the implementations of the topological indices.

2 Results and discussions

As far as MOF is concerned, Awais et al. (2020) studied the TI's of MOF based on it connectivity. The obtained results of TIs are analysed using 3D plots and in tabular form. Also Ali et al. (2020) studied the TIs of graph obtained as a graph operation namely T-sum graph. As far as dendrimers are concerned, ones that are have been discussed frequently are siloxan, POPAM and Trizan based dendrimers, see Igbal et al. (2020). In the same manner, Gao et al. (2020) discussed the entire classes of zagrab indices of two classes of Trizan dendrimers. The multiplicative Zagreb indices of planar octahedral networks namely planar octahedron network, triangular prism network and hex planar octahedron network are studied in Dustigeer et al. (2020). Moreover, the multiplicative Zagreb indices discussed in their aforementioned article are second multiplicative Zagreb index, first and second universal Zagreb indices, first and second hyper Zagreb indices, and sum and product connectivity indices. Manzoor et al. (2020) discussed entropy of carbon nano sheets using degree based TIs. They have discussed the obtained results in terms of 3D plots and tabular form.

Now, we discuss the research articles on the nexus of algebraic graph theory, chemical graph theory and computational graph with the referece of various molecular structures. The forgotten co-index of non-toxic dendrimers is discussed in Ali et al. (2021). Topological properties of some chemical networks, ceria oxide, subdivision of Sierpinki and hieriarchical hypercubes have been discussed in Bokhary et al. (2021b), Siddiqui et al. (2021a), Liu et al. (2021), and Zahra and Ibrahim (2021), respectively. Degree based TIs of caboxyterminated dendritic macromolecule has been studies by Rao et al. (2021). Szeged-type indices of SVE-join has been discussed in Asghar et al. (2021). Similarly, the topological properties of metal organic networks are studied in Chu et al. (2021) and Kashif et al. (2021). Moreover, the modified zagrab indices of random structures and the vertex PI index of certain triangular tessellation networks have been studied in Li et al. (2021) and Bokhary et al. (2021a). The ecentricity based properties of face centered cubic lattice are given in Shaker et al. (2021).

As far as algebraic graph theory and fluid mechanics is concerned, the thermodynamic properties cuboctahedral bi-metallic structure and the Hosoya properties of the commuting graph associated with the

group of symmetries have been studied in Siddiqui et al. (2021b) and Abbass et al. (2021). Moreover, computational graph theory is concerned with the computing results of the fractional metric dimension of metal organic frameforks in Raza et al. (2021), Liu et al. (2019), and Javaid et al. (2020).

Conflict of interest: Both authors (Muhammad Javaid and Muhammad Imran) are Guest Editors of the Main Group Metal Chemistry's Special Issue "Topological descriptors of chemical networks: Theoretical studies" in which this Editorial is published.

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