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Topological Indices Of Zero Divisor Graphs And Their Compliments

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ABSTRACT: Chemical graph theory is an area of mathematics that deals with the non-trivial applications of molecular problems. Chemical graph theory is an interdisciplinary science that studies molecular structures using graph theory and attempts to identify structural features involved in structure–property activity relationships using tools from graph theory, set theory, and statistics [1,2,3]. The topological characterization of chemical structures with the desired properties can be used to classify molecules and model unknown structures. In recent decades, much research has been conducted in this field. The topological index is a numerical value associated with chemical structures that purport to link chemical structures to various physicochemical properties, chemical reactivity, or biological activity. Topological indices are based on transforming a molecular graph into a number that describes the topology of the molecular graph [4,5,6,7]. Molecular modeling investigates the relationship between a chemical compound's structure, properties, and activity. Molecular graphs are frequently used to represent molecules and molecular compounds. A chemical graph is a model for describing the properties of a chemical compound. A molecular graph is a simple graph with vertices representing atoms and edges representing bonds. It can be represented by a drawing, a polynomial, a series of numbers, a matrix, or a derived number known as a topological index, which was first introduced by Wiener [8] in 1947.

KEYWORDS-topological, indices, zero, divisor, graphs, compliments

I. INTRODUCTION

The linear combination of the forgotten topological index and the first Zagreb index gives a mathematical model of certain physico-chemical properties of alkanes with high accuracy [14]. Randić observed the correlation between the Randic index and physio-chemical properties of alkane such as boiling point, enthalpy of formation, surface area, and so on. The strategy of encoding information on the molecular structure using topological indices has a low computational cost and a high predictive potential. Furthermore, these molecular descriptors provide insights about structural characteristics that are easily identified. The study of graphs built from commutative rings[1,2,3] focuses on the interaction between the algebraic and graph theoretical properties of the associated graph. This connection is applicable to information in communication theory. It is therefore worthwhile to compute the topological indices of the total graph and the zero divisor graph of the commutative ring.

Algebraic structures were investigated separately because of their strong links to representation theory and number theory, as well as their widespread use in combinatorics [2,3]. As a result of extensive mathematical research in this area,[4,5,6] finite rings and fields have received a significant amount of focus for their applications to cryptography and coding theory.

The technique of encoding information using topological molecular descriptors on the molecular structure has a low computational cost and a good predictive potential. Moreover, these molecular descriptors give ideas about structural characteristics with easy identification[7,8,9]

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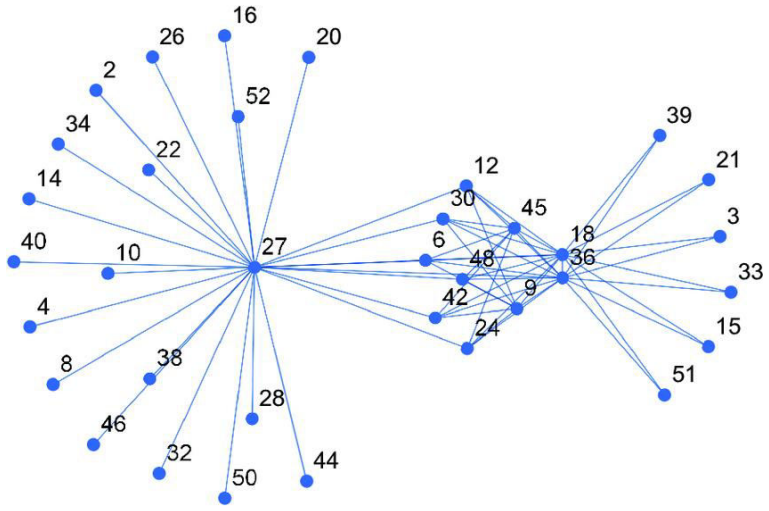

The zero-divisor graph G(Z 3 3 ×2)

The graphical invariant is considered as a structural invariant related to a graph. In molecular graph theory, the topological index is constructed as a graphical invariant. For this reason, the computing of topological indices of many graph structures has been an attractive research area for scientists especially chemists and mathematicians for a long time. Topological indices play an important role in mathematical chemistry such as the QSPR/QSAR modeling [10,11,12]. The Wiener index which is the oldest topological index and a distancebased index was studied for zero-divisor graphs in [10, 41, 47]. In 1972, the first Zagreb index and the second Zagreb index of graph G were suggested by Gutman and Trinajsti´c [13,14,15]. We attain more recent results on Zagreb index in [5, 7, 12, 13, 15,]. In 1975, Randi´c introduced the Randi´c index of a graph G [16,17,18]. Fajtlowicz proposed two topological indices which are called the harmonic index and the inverse degree index [18]. Furtula and Gutman introduced the forgotten topological index [21]. In 2020, the Sombor index of a graph G is defined by the mathematical chemist Ivan Gutman [24]. Then, Cruz et al. examine graphs extremal over the set of all chemical graphs, connected chemical graphs, chemical trees, and hexagonal systems using the Sombor index [14]. The Sombor index can be used successfully on modeling thermodynamic properties of compounds demonstrated by Red˘zepovi´c [19,20,21]. Alikhani et al. consider Sombor index of polymer graphs and show that the Sombor index of some graphs is computed from their monomer units [6]. The Sombor index has attracted important consideration from researchers within a very short time and many results about it can be found.

II. DISCUSSION

Graph constructing algorithms and their mapping with real life problems for scientific data analysis are getting popular. Standard algorithms construct the graph in a way that it can deal with all possibilities of input data to calculate the desired output. This article gives an algorithmic computational model for edge based eccentric topological indices by constructing zero divisor graph containing finite rings as Zp1p2 × Zq and Zp2 × Zq, where p, p1, p2 and q are primes numbers. At first algorithm classify vertices with common eccentricity and then computes first Zagreb, third Zagreb, geometric-arithmetic, atom-bond connectivity and harmonic index for zero divisor graphs containing commutative rings. Results of algorithms are verified using mathematical formulation so algorithm can be reuse or modify for applications of coding theory, algebraic cryptography, ICT, biology and chemistry easily.[19,20,21]

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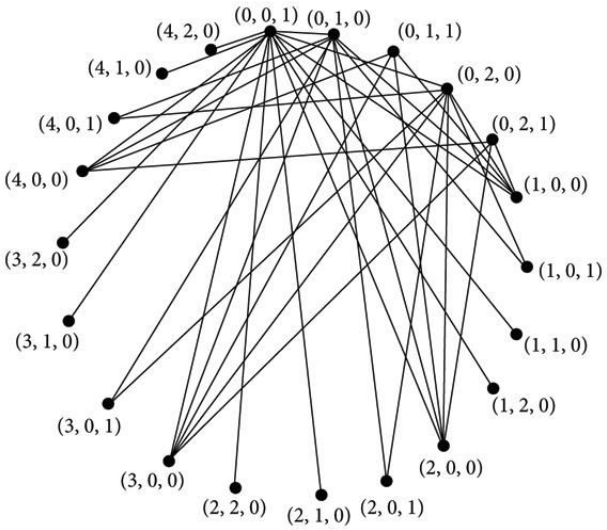

Topological Indices of Total Graph and Zero Divisor Graph of Commutative Ring: A Polynomial Approach

Graphs structures as powerful tool of formal science is facilitating the deep and innovative research in pure sciences, particularly in the field of chemistry and biology. This strong relation of graph theory with pure sciences has evolved interdisciplinary fields like molecular graph theory and biological networks. Many other practical problems can be represented and solved using graphs by emphasizing their applications in real world. Chemical graph theory incorporate, investigation of particles and atoms where graph structures are used to model pair wise relationship between objects. In last two decades many graph invariants have been studied and used for correlation analysis in theoretical chemistry, pharmacology, toxicology, and environmental chemistry [10]. Topological index is a numerical parameter of a graph which characterize it's topology and considered as a graph invariant. In the study of chemical graph theory, topological indices are used in the development of quantitative structure-activity relationship (QSARs) in which the properties of molecules are correlated [7, 9]. A variety of topological indices are available and have application in chemical graph theory , computer networks, statistics, physics, robotics and biological networks [22]. Topological indices can be classified as "degree based topological indices" [1, 21] and "distance based topological indices" [28, 13] on the basis of their dealing with degree of vertices or distance between the vertices. Some well-known degree based topological indices are Zagreb indices [19], atom bond connectivity [15] , geometric arithmetic index [20] , Randi connectivity index [23], Harmonic index [24] and sum connectivity index. Similarly distance based topological indices are Wiener index, Hosaya index, the energy and Estrada index [20,21]. Group and ring theory have been studied extensively for their close relationship with algebra, number theory and representation theory but also for their applications to other areas [6, 11]. Finite commutative rings is a part of group and ring theory. Now a days, finite commutative rings gain importance in many fields like algorithm analysis, engineering, combination theory, cryptography, coding theory, wireless communications, graph and iterative coding, data analysis and modeling, and finite geometry. Zero divisor graph is one of the important finite commutative rings [5, 6]. Topological indices as molecular descriptors have achieved an important place in the field of chemistry, pharmaceutical science. Moreover these indices have wide applications in nanotube structures [21]. Analysis of topological indices for a particular graph helps us to understand graph characteristics, their similarities and their differences with respect to the other graphs. Topological indices guide us that how the chemical structure can further grow and what COMPUTATION OF EDGE-BASED TOPOLOGICAL INDICES FOR ZERO DIVISOR ... 525 mathematical operations on the graphs with the help of topological indices can extend multidisciplinary research. 2. Definitions and notations For a connected graph G with

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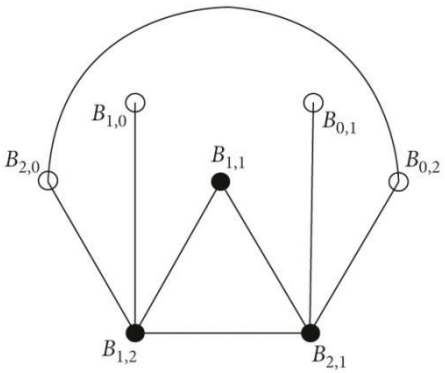
vertex and edge sets V (G) and E(G) respectively, a numerical quantity that is invariant under graph automorphisms is called topological index or topological descriptor. For a graph G the degree of a vertex v is the number of edges incident with v and is denoted by d(v). The maximum degree of a graph G, denoted by Δ(G), and the minimum degrees of a graph, denoted by δ(G). [18,19]

III. RESULTS

Graph theory has provided chemists with a variety of useful tools, such as topological indices. In terms of theoretical chemistry it is known as a graph invariant which predicts the chemical properties of the molecule.



Distance-Based Topological Polynomials Associated with Zero-Divisor Graphs

Note that every molecule can be modified as a graph by representing atoms as vertices and chemical bonds as edges. There are two major classes of topological indices namely distance-based topological indices and degree-based topological indices of graphs. These classes of topological indices are widely applied in chemistry and pharmacology. The concept of topological index came from the work done by Wiener [25] while he was working on the boiling point of paraffin. He named this index as path number. Later on, the path number was renamed as the Wiener index. The Wiener index is mostly used to determine structure–property relationships. In particular, the Wiener index has a variety of applications in pharmaceutical science and in the structure of nanotubes. For results and applications of Wiener index. On the other hand, the study of algebraic structures, using the properties of graph theory, tends to be an exciting research topic in the last two decades. The idea of the graph associated with zero-divisors of a commutative ring was introduced by Beck [6] in 1988. But, the present definition along with the name for the zero-divisor graph was first introduced by Anderson and Livingston in 1999.[17,18,19]

IV. CONCLUSION

For a commutative ring , the total graph of which denoted by , is a graph with all elements of R as vertices, and two distinct vertices are adjacent if and only if the set of zero-divisors of R. In an earlier study, we computed Wiener, hyper-Wiener, reverse Wiener, Randic´, Zagreb, and indices of zero-divisor graph. In this study, some computer programs are prepared to calculate the zero-divisors and adjacency matrix of the given graph which, apply these programs to compute the energy and first edge-Wiener, sum-connectivity, harmonic, augmented Zagreb and hyper-Zagreb indices.[19,20,21]

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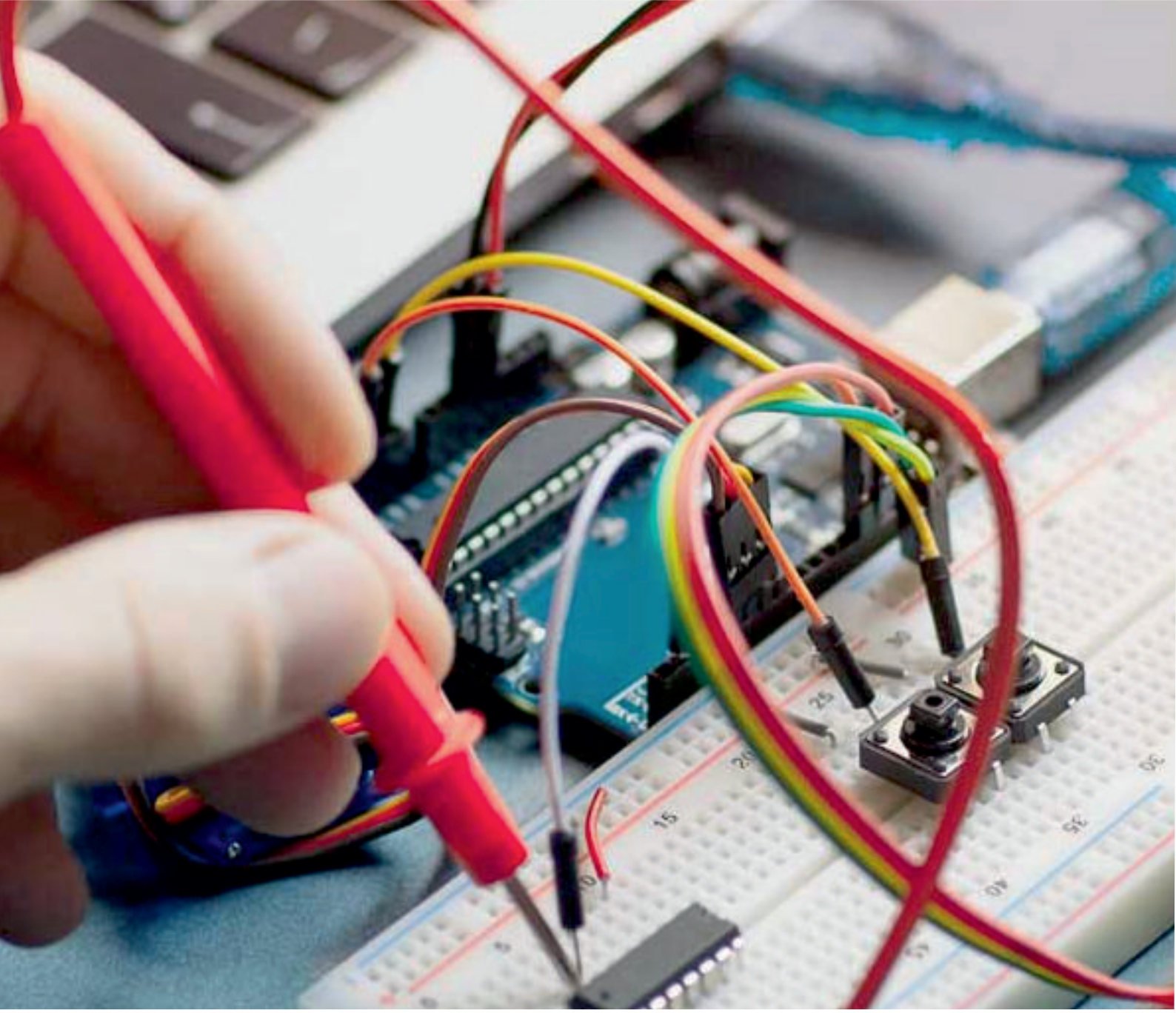

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