Preface

This volume is the Pre-conference Proceedings of the Second International Conference on Algebra and Discrete Mathematics (ICADM-2020) conducted by the Department of Mathematics, DDE, Madurai Kamaraj University during June 24 -26, 2020 in online mode. The main themes of the conference are Algebra, Discrete Mathematics and their applications. The role of Algebra and Discrete Mathematics in the field of Mathematics has been rapidly increasing over several decades. In recent decades, the graphs constructed out of algebraic structures have been extensively studied by many authors and have become a major field of research. The benefit of studying these graphs is that one may find some algebraic property of the under lying algebraic structure through the graph property and the vice-versa. The tools of each have been used in the other to explore and investigate the problem in deep. This conference is organized with the aim of providing an avenue for discussing recent advancements in these fields and exploring the possibility of effective interactions between these two areas.

The aim of the conference is to introduce research topics in the main streams of Algebra and Discrete Mathematics to young researchers especially research students, and encourage them to collaborate in teams lead by well-known mathematicians from various countries.

This volume makes available a record of articles presented in the conference. This volume contains the papers presented in the conference without any referring process.

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Some topological indices of Molybdenum disulfide

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Abstract

This paper aims at deriving formula for various topological indices for Molybdenum disulfide (MoS2) nanostructure. Various topological indices which are frequently studied for establishing correlation between chemical structural information and physical properties are derived for MoS2 nanostructure. The topological indices are first, second, third and modified Zagreb indices and various connectivity indices namely Randic index, ABC index, Sum connectivity index, geometric-arithmetic index.

Keywords: Molybdenum disulfide,topological index, Zagreb indices, connectivity indices.

1 Introduction

In theoretical chemistry topological indices are used for studying the physical, biological properties of the chemical compounds and they are used to predict certain physicochemical properties like boiling point, stability, enthalpy of vaporization and so forth. There are certain types of topological indices such as degree based topological indices, distance based topological indices and counting related topological indices etc. Among degree based topological indices, the so-called Zagreb indices, atom-bond connectivity (ABC), Randic index, Sum connectivity index, geometric–arithmetic (GA) are of vital importance.

The MoS_2 (Molybdenum disulphide) is an inorganic compound with layered structure where a plane of Molybdenum atoms is sandwiched by planes of sulfide ions. As it has a low friction and robustness, it is used as a lubricant and it is also used as co-catalyst. The Schematic representation of side view of a monolayer of MoS2 is shown in figure(1) and top view graphical representation is given in figure(2). The layered structure makes it to be used as lubricant, capable of handling shear stress.

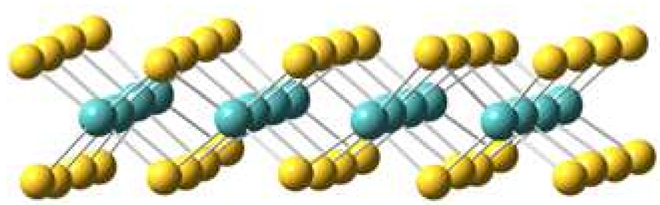

Figure 1: Schematic representation of side view of a monolayer of MoS_2

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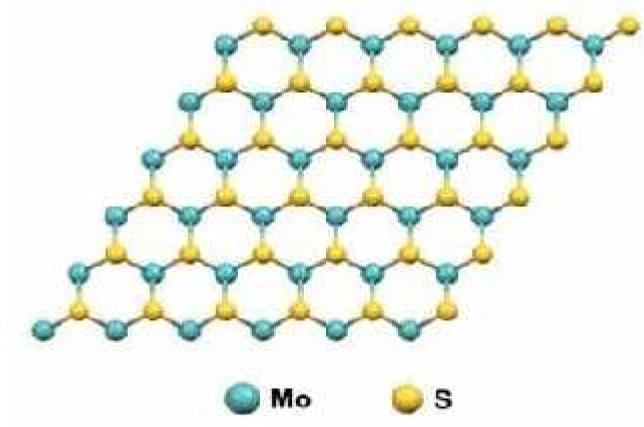

Figure 2: Top view graphical representation of MoS_2

1.1 Definitions

A graph G is an ordered pair (V, E), where V is the set of vertices and E is the edge set. The edge connecting the vertex u and vertex v is denoted by uv. The degree of a vertex v is denoted by d_v, For additional notations the reader may refer to [7].
Zagreb indices were first defined by Gutman and Trinajstic[8] in studying pi-electron energy of compounds. For graph G the definitions of Zagreb indices are given below:

$$First\ Zagreb\ index: \qquad M_1(G) = \sum_{uv \in E} (d_u + d_v) \tag{1}$$

$$Second\ Zagreb\ index: \qquad M_2(G) = \sum_{uv \in E} (d_u.d_v) \tag{2}$$

$$Third\ Zagreb\ index: \qquad M_3(G) = \sum_{uv \in E} |d_u - d_v| \tag{3}$$

$$Modified\ Zagreb\ index: \qquad M_2^*(G) = \sum_{uv \in E} \frac{1}{d_u.d_v} \tag{4}$$

1.2 Connectivity Indices

Connectivity indices are topological descriptor having applications in theoretical chemistry. The first and oldest degree based topological index is Randic index[11].It provides a quantitative assessment of branching of molecules.The Randic index (product-connectivity index) is defined as

$$R_{-\frac{1}{2}}(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u.d_v}} \tag{5}$$

The atom-bond connectivity index(ABC index), is one of the degree based molecular descriptors, which was introduced by Estrada et al. [5] in late 1990s, and it can be used for modelling thermodynamic properties of organic chemical compounds; it is also used as a tool for explaining the stability of branched alkanes [6]. Some upper bounds for the atom bond connectivity index of graphs can be found in[10]. For further results on ABC index of trees, see the papers[1] [12][13]and the references cited therein. Atom-Bond Connectivity (ABC) index of a graph G is defined as

$$ABC(G) = \sum_{uv \in E} \sqrt{\frac{d_u + d_v - 2}{d_u.d_v}} \tag{6}$$

Sum connectivity index belongs to a family of Randic like indices and it was introduced by Zhou and Trinajstic [2]. Further studies on Sum connectivity index can be found in [3]. Sum-connectivity index is defined as

$$X(G) = \sum_{uv \in E} \frac{1}{\sqrt{(d_u + d_v)}} \tag{7}$$

Vukicevic and Furtula defined degree based topological index called Geometric- Arithmetic index[4] as

$$GA(G) = \sum_{uv \in E} \frac{2\sqrt{d_u d_v}}{(d_u + d_v)} \tag{8}$$

1.3 Different types of edges in MoS_2

The MoS2 structural graph is shown in figure. Based on the that there are three types of edges, one connecting vertex with degree two to another vertex with degree two, second type of edge connects vertex with degree two to vertex with degree four and the third type of vertex connects vertex with degree four to vertex with degree four. The number of edges for each type of edges for MoS_2 is given in the table below.

(d_u, d_v)	$(2,2)$	(2,4)	(4,4)
No. of edges	4	$4p + 4q - 8$	$4pq - 4p - 4q + 4$

Table 1: Edge partition in MoS_2

2 Results

THEOREM 1. *The Zagreb indices for MoS_2 are given by*

(i) $M_1(MoS_2) = 32pq - 8p - 8q$

(ii) $M_2(MoS_2) = 64pq - 32p - 32q + 16$

(iii) $M_3(MoS_2) = 8p + 8q - 16$

(iv) $M_2^*(MoS_2) = \frac{1}{4}(pq + p + q + 1)$

Proof. (i) from (1) , $M_1(G) = \sum_{uv \in E} (d_u + d_v)$

using table(1) we get

$$M_1(MoS_2) = 4(2+2) + (4p + 4q - 8)(2+4) + (4pq - 4p - 4q + 4)(4+4)$$
$$\therefore M_1(MoS_2) = 32pq - 8p - 8q$$

(ii) from (2), $M_2(G) = \sum_{uv \in E} (d_u.d_v)$

using table(1) we get

$$M_2(MoS_2) = 4(2.2) + (4p + 4q - 8)(2.4) + (4pq - 4p - 4q + 4)(4.4)$$
$$\therefore M_2(MoS_2) = 64pq - 32p - 32q + 16$$

(iii) from (3), $M_3(G) = \sum_{uv \in E} |d_u - d_v|$

using table(1) we get

$$M_3(MoS_2) = 4|2-2| + (4p+4q-8)|2-4| + (4pq-4p-4q+4)|4-4|$$
$$\therefore M_3(MoS_2) = 8p+8q-16$$

(iv) from (4), $M_2^*(G) = \sum_{uv \in E} \frac{1}{d_u.d_v}$

using table(1) we get

$$M_2^*(MoS_2) = 4\left(\frac{1}{2.2}\right) + (4p+4q-8)\left(\frac{1}{2.4}\right) + (4pq-4p-4q+4)\left(\frac{1}{4.4}\right)$$
$$\therefore M_2^*((MoS_2) = \frac{1}{4}(pq+p+q+1)$$

□

THEOREM 2. *The Connectivity indices are given by*

(i) $R_{-\frac{1}{2}}(MoS_2) = pq - 0.4142(p+q) + 0.1716$

(ii) $ABC(MoS_2) = \sqrt{6}pq + 0.3789(p+q-1)$

(iii) $X(MoS_2) = \sqrt{2}pq + 0.2188(p+q) + 0.1482$

(iv) $GA(MoS_2) = 4pq - 0.2288(p+q-2)$

Proof. (i) from (5) , $R_{-\frac{1}{2}}(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u.d_v}}$

using table(1) we get

$$R_{-\frac{1}{2}}(MoS_2) = 4\left(\frac{1}{\sqrt{2.2}}\right) + (4p+4q-8)\left(\frac{1}{\sqrt{2.4}}\right) + (4pq-4p-4q+4)\left(\frac{1}{\sqrt{4.4}}\right)$$
$$\therefore R_{-\frac{1}{2}}(MoS_2) = pq - 0.4142(p+q) + 0.1716$$

(ii) from (6), $ABC(G) = \sum_{uv \in E} \sqrt{\frac{d_u + d_v - 2}{d_u.d_v}}$

using table(1) we get

$$ABC(MoS_2) = 4\sqrt{\frac{2+2-2}{2.2}} + (4p+4q-8)\sqrt{\frac{2+4-2}{2.4}} + (4pq-4p-4q+4)\sqrt{\frac{4+4-2}{4.4}}$$
$$\therefore ABC(MoS_2) = \sqrt{6}pq + 0.3789(p+q-1)$$

(iii) from (7), $X(G) = \sum_{uv \in E} \frac{1}{\sqrt{(d_u + d_v)}}$

using table(1) we get

$$X(MoS_2) = 4\left(\frac{1}{\sqrt{2+2}}\right) + (4p+4q-8)\left(\frac{1}{\sqrt{2+4}}\right) + (4pq-4p-4q+4)\left(\frac{1}{\sqrt{4+4}}\right)$$
$$\therefore X(MoS_2) = \sqrt{2}pq + 0.2188(p+q) + 0.1482$$

(iv) from (8), $GA(G) = \sum_{uv \in E} \frac{2\sqrt{d_u d_v}}{(d_u + d_v)}$
using table(1) we get

$$GA(MoS_2) = 4\left(\frac{2\sqrt{2.2}}{2+2}\right) + (4p + 4q - 8)\left(\frac{2\sqrt{2.4}}{2+4}\right) + (4pq - 4p - 4q + 4)\left(\frac{2\sqrt{4.4}}{4+4}\right)$$

$$\therefore GA((MoS_2) = 4pq - 0.2288(p + q - 2)$$

□

3 Conclusion

The problem of finding the general formula for Zagreb indices, ABC index, Randic connectivity index, Sum connectivity index and GA index of Molybdenum disulfide (MoS2) nanostructure is solved here analytically without using computers.

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