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ORIGINAL ARTICLE

Topological aspects of metal-organic structure with the help of underlying networks

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Abstract Metal–organic structures/Networks (MONs) are useful in modern chemistry. It is common to use as a storehouse for the storage of gases, it plays a role in the separation of gases and purification. The most important feature of MONs is that it acts as a predecessor for the development of a large number of nanostructures. Furthermore, MONs reflect very useful chemical-physical properties, changing organic ligands, exchanging of ions, etc. The method used to forecast the natural behaviors among the chemical-physical specifications of the chemical compounds in their primitive network is known as topological indices or TIs. This numerical quantity is used in the method of forecasting. *TIs* of MONs shows a key role in the environmental and theoretical pharmacology and chemistry. Line graphs also have powerful applications in chemistry and predicting the boiling point of cycloalkanes. In this paper, we study Randić, atom bound connectivity, geometric arithmetic, Zagreb, Multiplicative Zagreb, redefined Zagreb indices and Zagreb coindices for line graph of first organic network $L(MON_1(\chi))$ and second organic network $L(MON_2(\chi)), \chi \geqslant 2$.

1. Introduction

Graph theory plays a significant role in modern chemistry. In chemical graph theory, the atoms of molecules referred to as vertices, and chemical bonds between atoms referred to as edges. Graph theory provides the fundamentals tools to predict the properties of chemical networks. A topological index is a special tool that is used to describes the properties of chemical networks such as melting, flash and boiling points, temperature, tension, pressure, retention times, partition coefficient, the heat of formation, the heat of evaporation, and density

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(Matamala and Estrada, 2005; Rker and Rücker, 1999; Diaz et al., 2007; Gutman, 1994). Topological indices (TIs) are also associated with quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) (Devillers et al., 1997; Gutman and Polansky, 1986). Degree-based and distance-based are the two major TIs. First time in 1957, Wiener used the distance-based TI to compute the boiling points of paraffin (Wiener, 1947).

There are many research work related to TIs most recent are following, on the edge dividing method implemented for a molecular structure (Gao and Farahani, 2015) discussed by Gao and Farahani, Gao et al. and Shao et al. discussed several atom bond analysis in Gao et al. (2016), Shao et al. (2018), topological indices on a network of honeycomb Hayat et al. (2015) studied by Hayat et al., reverse method of computing topological indices implemented in Gao et al. (2018), Nadeem et al. (2016), computed TIs of the line graphs of two-dimensional lattice, nanotorus and nanotube of $TUC_4C_8[p,q]$ with the operation of subdivision. Shabbir et al. (2020), worked on the two different nanotubes and computed the edge version of degree-based TIs. Baig et al. (2015), computed the TIs of poly-oxide, poly-silicate, DOX, and DSL networks. Nadeem et al. (2019), calculated the TIs of para-line graphs of V-phenylene nanostructures. Gutman and Estrada (1996) studied the TIs of the acyclic molecular graph and as well as on the line graph of the acyclic molecular graph and observed that the Wiener index (WI) of the molecular graph and the WI of the line graph differ by just a constant, some recent article on different topological indices and considering chemical structures we refer (Guirao et al., 2020; Cai et al., 2020; Jahanbani et al., 2020; Nadeem et al., 2019; Shabbir et al., 2020; Zheng et al., 2020).

In 2019, Wasson et al. (2019) proposed the idea of linker competition with a framework of metal–organic network (MON) for the topological perspectives. Furthermore, a fast hydrogen detecting device introduced by Tea et al. (2017) containing organic ligands and metal recognized as the metal–organic network (MON) which is able to identify the molecular hydrogen stages within seven seconds when it will be less than one percent.The MONs also show the physical and chemical properties such as changing organic ligands (Eddaoudi, 2002) and post-synthetic ligand (Min et al., 2012). The MONs are very useful devices for storage, the forerunner for the formation of many nano-structures (Min et al., 2017).

Let Υ be a simple, without loop and connected molecular graph with vertex set $V(\Upsilon)$ and edge set $E(\Upsilon)$. Let the order of molecular graph is $V(\Upsilon) = n$ and size is $E(\Upsilon) = m$. The degree $\zeta(a)$ of a vertex a is a total number of vertices adjacent to a. A line graph $L(\Upsilon)$ of graph Υ is a graph that having order m and two vertices $x, y \in V(\Upsilon)$ having common neighborhood in $L(\Upsilon)$ iff their corresponding edges are adjacent in Υ.

2. Methodology of computing topological indices

The concept of a line graph is not very new in chemical graph theory and the applications of line graph can be found in chemistry such as quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) could be developed on the basis of TIs of line graph (Gutman and Tomovic, 2000), predict the boiling points of Cyclone-alkalies (Gutman and Tomovic, 2001), and predicting the surface tension of alkanes (Gutman et al., 1997). Following are some of the formulas of topological indices which are discussed in this work along with their citations.

The *Randić* index (R_α) (Randić, 1975) for a graph Υ defined as:

$$R_\alpha(\Upsilon) = \sum_{ab\in E(\Upsilon)} (\zeta(a)\times\zeta(b))^\alpha. \tag{1}$$

The atom bond connectivity index (ABC) (Estrada et al., 1998) and geometric arithmetic index (GA) (Vukičević and Furtula, 2009) for a graph Υ defined as:

$$ABC(\Upsilon) = \sum_{ab\in E(\Upsilon)} \sqrt{\frac{\zeta(a)+\zeta(b)-2}{\zeta(a)\times\zeta(b)}}, \tag{2}$$

$$GA(\Upsilon) = \sum_{ab\in E(\Upsilon)} \frac{2\sqrt{\zeta(a)\times\zeta(b)}}{\zeta(a)+\zeta(b)} \tag{3}$$

The first and second Zagreb index is introduced in 1972 (Gutman and Trinajstć, 1972; Gutman and Das, 2004) and hyper-Zagreb index (Shirdel et al., 2013) for a graph Υ defined as:

$$M_1(\Upsilon) = \sum_{ab\in E(\Upsilon)} (\zeta(a)+\zeta(b)), \tag{4}$$

$$M_2(\Upsilon) = \sum_{ab\in E(\Upsilon)} (\zeta(a)\times\zeta(b)), \tag{5}$$

$$HM(\Upsilon) = \sum\nolimits_{ab\in E(\Upsilon)} [\zeta(a)+\zeta(b)]^2 \tag{6}$$

The first and second Zagreb coindices defined in 2008 (Došlić, 2008) for a graph Υ defined as:

$$\overline{M_1} = \overline{M_1}(\Upsilon) = \sum_{ab\notin E(\Upsilon)} [\zeta(a)+\zeta(b)], \tag{7}$$

$$\overline{M_2} = \overline{M_2}(\Upsilon) = \sum_{ab\notin E(\Upsilon)} (\zeta(a)\times\zeta(b)). \tag{8}$$

Let Υ be a graph with n vertices and m edges (Gutman et al., 2015). Then

$$\overline{M_1}(\Upsilon) = 2m(n-1) - M_1(\Upsilon), \tag{9}$$

$$\overline{M_2}(\Upsilon) = 2m^2 - \frac{1}{2}M_1(\Upsilon) - M_2(\Upsilon). \tag{10}$$

The first and second multiplicative Zagreb indices (Ghorbani and Azimi, 2012) for a graph Υ defined as:

$$PM_1(\Upsilon) = \prod_{ab\in E(\Upsilon)} [\zeta(a)+\zeta(b)], \tag{11}$$

$$PM_2(\Upsilon) = \prod_{ab\in E(\Upsilon)} [\zeta(a)\times\zeta(b)]. \tag{12}$$

The Forgotten (Furtula and Gutman, 2015), Augmented Zagreb (Furtula et al., 2010), and Balaban (Balaban, 1982, 1983) for a graph Υ defined as:

$$F(\Upsilon) = \sum_{ab\in E(\Upsilon)} \left(\zeta(a)^2+\zeta(b)^2\right), \tag{13}$$

$$AZI(\Upsilon) = \sum_{ab\in E(\Upsilon)} \left(\frac{\zeta(a)\times\zeta(b)}{\zeta(a)+\zeta(b)-2}\right)^3, \tag{14}$$

$$J(\Upsilon) = \frac{m}{m-n+2} \sum_{ab\in E(\Upsilon)} \frac{1}{\sqrt{\zeta(a)\times\zeta(b)}.} \tag{15}$$

The redefined first, second and third Zagreb indices (Ranjini et al., 2013) for a graph Υ defined as;

$$ReZG_1(\Upsilon) = \sum_{ab \in E(\Upsilon)} \frac{\zeta(a) + \zeta(b)}{\zeta(a) \times \zeta(b)}, \quad (16)$$

$$ReZG_2(\Upsilon) = \sum_{ab \in E(\Upsilon)} \frac{\zeta(a) \times \zeta(b)}{\zeta(a) + \zeta(b)}, \quad (17)$$

$$ReZG_3(\Upsilon) = \sum_{ab \in E(\Upsilon)} \zeta(a) \times \zeta(b)(\zeta(a) + \zeta(b)). \quad (18)$$

The remaining paper categorized as, Section 2, computations the TIs and co-indices of the line graphs of first metal–organic network $L(MON_1(\chi))$ and in Section 3, we computed TIs and co-indices of the line graphs of second metal–organic network $L(MON_2(\chi))$.

3. Results of the Topological Indices of line graph of organic network $L(MON_1(\chi))$

In this section, we will discuss about line graph of first metal–organic network $MON_1(\chi)$. The first metal organic network discussed in Hong et al. (2020) and line graph of first organic network $L(MON_1(2))$ is shown in Fig. 1. In this paper, we represents the line graph of metal organic network $L(MON_1(\chi))$ as Υ_1. The order of $L(MON_1(\chi))$ is $n_1 = V(\Upsilon_1) = 72\chi - 12$ and size of $L(MON_1(\chi))$ is $m_1 = E(\Upsilon) = 192\chi + 98$. There are seven different types of edges in Υ_1 on the bases of different degree of end vertices. We have

$$\begin{aligned} E_1(3,3) &= \{ab \in E(\Upsilon_1(\chi)) | \zeta(a) = 3, \zeta(b) = 3\}, \\ E_2(3,6) &= \{ab \in E(\Upsilon_1(\chi)) | \zeta(a) = 3, \zeta(b) = 6\}, \\ E_3(4,4) &= \{ab \in E(\Upsilon_1(\chi)) | \zeta(a) = 4, \zeta(b) = 4\}, \\ E_4(4,8) &= \{ab \in E(\Upsilon_1(\chi)) | \zeta(a) = 4, \zeta(b) = 8\}, \\ E_5(6,8) &= \{ab \in E(\Upsilon_1(\chi)) | \zeta(a) = 6, \zeta(b) = 8\}, \\ E_6(6,6) &= \{ab \in E(\Upsilon_1(\chi)) | \zeta(a) = 6, \zeta(b) = 6\}, \\ E_7(8,8) &= \{ab \in E(\Upsilon_1(\chi)) | \zeta(a) = 8, \zeta(b) = 8\}. \end{aligned} \quad (19)$$

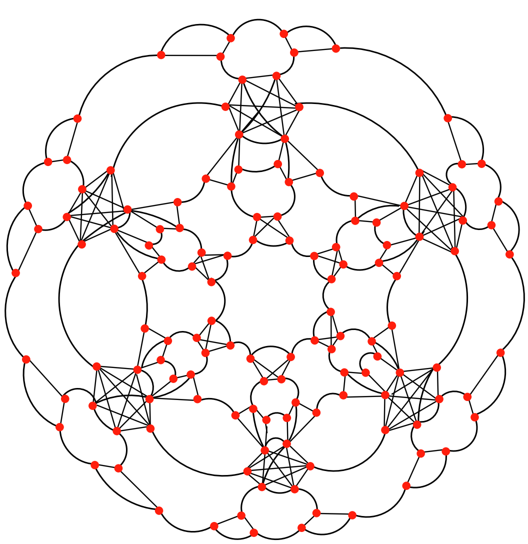

Fig. 1 Line grapph of metal–organic network $L(MON_1(2))$.

where

$$\begin{aligned} |E(\Upsilon_1)| &= |E_1| + |E_2| + |E_3| + |E_4| + |E_5| + |E_6| + |E_7|, \\ &= 48 + 12(\chi - 1) + 50 + 30(\chi - 1) + 36(\chi - 1) \\ &\quad + 48(\chi - 1) + 60(\chi - 1) + 6(\chi - 1), \\ &= 192\chi + 98. \end{aligned} \quad (20)$$

Theorem 3.1. *Let $\Upsilon_1 \cong L(MON_1(\chi))$ be a line graph of first metal–organic compound network with $\chi \geqslant 2$. Then general Randić indices are*

$$\begin{aligned} &1: R_1(\Upsilon_1) = 6697\chi - 5465, \\ &2: R_{-1}(\Upsilon_1) = 6.42708\chi + 2.03122, \\ &3: R_{\frac{1}{2}}(\Upsilon_1) = 1115.11219\chi - 771.1129, \\ &4: R_{-\frac{1}{2}}(\Upsilon_1) = 34.37059\chi - 5.87059. \end{aligned}$$

Proof. Using formula from Eqs. (1), (19) and (20), the general Randić indices are computed as bleow, for $\alpha = \pm 1, \pm \frac{1}{2}$,

$$\begin{aligned} R_1(\Upsilon_1) = &\ 48(9) + 12(\chi-1)(18) + (50 + 30(\chi-1))(16) + 36(\chi-1)(32), \\ &+ 6(\chi-1)(64) + 48(\chi-1)48 + 60(\chi-1)36, \\ = &\ (480 + 6216)(\chi-1) + 432 + 800 = 6697(\chi-1) + 1232 = 6697\chi - 5465. \\ R_{-1}(\Upsilon_1) = &\ 48(9)^{-1} + 12(\chi-1)(18)^{-1} + (50 + 30(\chi-1))(16)^{-1} + 36(\chi-1)(32)^{-1} \\ &+ 6(\chi-1)(64)^{-1} + 48(\chi-1)(48)^{-1} + 60(\chi-1)(36)^{-1}, \\ = &\ (4.55208 + 1.875)(\chi-1) + 3.125 + 5.333 = 6.42708(\chi-1) + 8.4583, \\ = &\ 6.42708\chi + 2.03122. \\ R_{\frac{1}{2}}(\Upsilon_1) = &\ 48(9)^{\frac{1}{2}} + 12(\chi-1)(18)^{\frac{1}{2}} + (50 + 30(\chi-1))(16)^{\frac{1}{2}} + 36(\chi-1)(32)^{\frac{1}{2}}, \\ &+ 6(\chi-1)(64)^{\frac{1}{2}} + 48(\chi-1)(48)^{\frac{1}{2}} + 60(\chi-1)(36)^{\frac{1}{2}}, \\ = &\ (995.11219 + 120)(\chi-1) + 344 = 1115.11219(\chi-1) + 344, \\ = &\ 1115.11219\chi - 771.1129. \\ R_{-\frac{1}{2}}(\Upsilon_1) = &\ 48(9)^{-\frac{1}{2}} + 12(\chi-1)(18)^{-\frac{1}{2}} + (50 + 30(\chi-1))(16)^{-\frac{1}{2}} + 36(\chi-1)(32)^{-\frac{1}{2}}, \\ &+ 6(\chi-1)(64)^{-\frac{1}{2}} + 48(\chi-1)(48)^{-\frac{1}{2}} + 60(\chi-1)(36)^{-\frac{1}{2}}, \\ = &\ 34.37059(\chi-1) + 28.5 = 34.37059\chi - 5.87059. \end{aligned}$$

□

Theorem 3.2. *Let $\Upsilon_1 \cong L(MON_1(\chi))$ be a line graph of first metal–organic compound network with $\chi \geqslant 2$. Then the atom bond connectivity and geometric arithmetic indices are;*

$$\begin{aligned} 1: ABC(\Upsilon_1) = 104.40731\chi - 41.7887, 2: GA(\Upsilon_1) \\ = 188.76242\chi - 90.76242. \end{aligned}$$

Proof. Using formulae from Eqs. (2), (3), (19) and (20), the atom bond connectivity and geometric arithmetic indices computed as below,

$$\begin{aligned} ABC(\Upsilon_1) &= 48\sqrt{\tfrac{3+3-2}{3\times3}} + 12(\chi-1)\sqrt{\tfrac{3+6-2}{3\times6}} + (50 + 30(\chi-1))\sqrt{\tfrac{4+4-2}{4\times4}}, \\ &+ 36(\chi-1)\sqrt{\tfrac{4+8-2}{4\times8}} + 6(\chi-1)\sqrt{\tfrac{8+8-2}{8\times8}} + 48(\chi-1)\sqrt{\tfrac{6+8-2}{6\times8}} \\ &+ 60(\chi-1)\sqrt{\tfrac{6+6-2}{6\times6}} \\ &= 104.40731(\chi-1) + 62.6186 = 104.40731\chi - 41.7887. \end{aligned}$$

$$\begin{aligned} GA(\Upsilon_1) &= 48\tfrac{2\sqrt{3\times3}}{3+3} + 12(\chi-1)\tfrac{2\sqrt{3\times6}}{3+6} + (50 + 30(\chi-1))\tfrac{2\sqrt{4\times4}}{4+4} \\ &+ 36(\chi-1)\tfrac{2\sqrt{4\times8}}{4+8} + 6(\chi-1)\tfrac{2\sqrt{8\times8}}{8+8} + 48(\chi-1)\tfrac{2\sqrt{6\times8}}{6+8} \\ &+ 60(\chi-1)\tfrac{2\sqrt{6\times6}}{6+6} = 188.76242(\chi-1) + 98 = 188.76242\chi - 90.76242. \end{aligned}$$

□

Theorem 3.3. *Let $\Upsilon_1 \cong L(MON_1(\chi))$ be a line graph of first metal–organic compound network with $\chi \geqslant 2$. Then the first, second Zagreb and hyper-Zagreb indices are,*

$$\begin{aligned} 1 &: M_1(\Upsilon_1) = 2268\chi - 1580, \\ 2 &: M_2(\Upsilon_1) = 10056\chi - 8824, \\ 3 &: HM(\Upsilon_1) = 96780\chi - 91852. \end{aligned}$$

Proof. Using formulae from Eqs. (4), (5), (6), (19), and (20) for the first, second Zagreb and hyper-Zagreb indices respectively.

$$\begin{aligned} M_1(\Upsilon_1) &= 48(3+3) + 12(\chi-1)(3+6) + (50+30(\chi-1))(4+4) + 36(\chi-1)(4+8) \\ &\quad + 6(\chi-1)(8+8) + 48(\chi-1)(6+8) + 60(\chi-1)(6+6), \\ &= 2268(\chi-1) + 688 = 2268\chi - 1580. \\ M_2(\Upsilon_1) &= 48(3\times 3) + 12(\chi-1)(3\times 6) + (50+30(\chi-1))(4\times 4) + 36(\chi-1)(4\times 8) \\ &\quad + 6(\chi-1)(8\times 8) + 48(\chi-1)(6\times 8) + 60(\chi-1)(6\times 6), \\ &= 10056(\chi-1) + 1232 = 10056\chi - 8824. \end{aligned}$$

$$\begin{aligned} HM(\Upsilon) &= 48(3+3)^2 + 12(\chi-1)(3+6)^2 + (50+30(\chi-1))(4+4)^2 + 36(\chi-1)(4+8)^2 \\ &\quad + 6(\chi-1)(8+8)^2 + 48(\chi-1)(6+8)^2 + 60(\chi-1)(6+6)^2, \\ &= 96780(\chi-1) + 4928 = 96780\chi - 91852. \end{aligned}$$

□

Theorem 3.4. *Let $\Upsilon_1 \cong L(MON_1(\chi))$ be a line graph of first metal–organic compound network with $\chi \geqslant 2$. Then the first and second Zagreb coindices are,*

$$\begin{aligned} 1 &: \overline{M_1}(\Upsilon_1) = 27648\chi^2 - 936\chi + 6276, \\ 2 &: \overline{M_2}(\Upsilon_1) = 73728\chi^2 - 48822\chi + 10302. \end{aligned}$$

Proof. Using formula from either Eqs. (7), (8) or (9), (10) with Eqs. (19) and (20), the first and second Zagreb coindex is computed as below,

$$\begin{aligned} \overline{M_1}(\Upsilon_1) &= 2\cdot(192\chi+98)\cdot(72\chi-13) - (10056(\chi-1)+1232), \\ &= 27648\chi^2 - 936\chi + 6276. \\ \overline{M_2}(\Upsilon_1) &= 2\cdot(192\chi+98))^2 - \tfrac{1}{2}(2268(\chi-1)+688) - (10056(\chi-1)+1232), \\ &= 73728\chi^2 - 48822\chi + 10302. \end{aligned}$$

□

Theorem 3.5. *Let $\Upsilon_1 \cong L(MON_1(\chi))$ be a line graph of first metal–organic compound network with $\chi \geqslant 2$. The first and second multiplicative Zagreb indices are*

$$\begin{aligned} 1 &: PM_1(\Upsilon_1) = 3^{120\chi-72}\cdot 2^{354\chi-156}\cdot 7^{48(\chi-1)} \\ 2 &: PM_2(\Upsilon_1) = 2^{660\chi-460}\cdot 3^{192\chi-96} \end{aligned}$$

Proof. Using formula from Eqs. (11), (12) with Eqs. (19), and (20) the first and second multiplicative Zagreb index is computed as:

$$\begin{aligned} PM_1(\Upsilon_!) &= (3+3)^{48}\times(3+6)^{12(\chi-1)}\times(4+4)^{(50+30(\chi-1))}\times(4+8)^{36(\chi-1)} \\ &\quad \times(8+8)^{6(\chi-1)}\times(6+8)^{48(\chi-1)}\times(6+6)^{60(\chi-1)}, \\ &= 6^{48}\cdot 9^{12(\chi-1)}\cdot 8^{(50+30(\chi-1))}\cdot 12^{36(\chi-1)}\cdot 16^{6(\chi-1)}\cdot 14^{48(\chi-1)}\cdot 12^{60(\chi-1)}, \\ &= 3^{120\chi-72}\cdot 2^{354\chi-156}\cdot 7^{48(\chi-1)}. \end{aligned}$$

$$\begin{aligned} PM_2(\Upsilon_1) &= (3\times 3)^{48}\times(3\times 6)^{12(\chi-1)}\times(4\times 4)^{(50+30(\chi-1))}\times(4\times 8)^{36(\chi-1)}\times(8\times 8)^{6(\chi-1)} \\ &\quad \times(6\times 8)^{48(\chi-1)}\times(6\times 6)^{60(\chi-1)}, \\ &= 9^{48}\cdot 18^{12(\chi-1)}\cdot 16^{(50+30(\chi-1))}\cdot 32^{36(\chi-1)}\cdot 64^{6(\chi-1)}\cdot 48^{48(\chi-1)}\cdot 36^{60(\chi-1)}. \\ &= 2^{660\chi-460}\cdot 3^{192\chi-96}. \end{aligned}$$

□

Theorem 3.6. *Let $\Upsilon_1 \cong L(MON_1(\chi))$ be a line graph of first metal–organic compound network with $\chi \geqslant 2$. Then the forgotten, augmented Zagreb and Balaban indices are,*

$$\begin{aligned} 1 &: F(\Upsilon_1) = 14268\chi - 11804, \\ 2 &: AZI(\Upsilon_1) = 237.9177\chi - 61.26464, \\ 3 &: J(\Upsilon_1) = \tfrac{192\chi+98}{120\chi+112}[34.37059(\chi-1)+28.5]. \end{aligned}$$

Proof. Putting Eqs. (19), (20) in the formula from Eqs. (13)–(15), the results computed as:

$$\begin{aligned} F(\Upsilon_1) &= 48(3^2+3^2) + 12(\chi-1)(3^2+6^2) + (50+30(\chi-1)) \\ &\quad \times(4^2+4^2) + 36(\chi-1)(4^2+8^2) + 6(\chi-1)(8^2+8^2) \\ &\quad + 48(\chi-1)(6^2+8^2) + 60(\chi-1)(6^2+6^2) \\ &= 14268(\chi-1) + 2464 = 14268\chi - 11804. \end{aligned}$$

$$\begin{aligned} AZI(\Upsilon_1) &= 48\left(\frac{3\times 3}{3+3-2}\right)^3 + 12(\chi-1)\left(\frac{3\times 6}{3+6-2}\right)^3 \\ &\quad + (50+30(\chi-1))\left(\frac{4\times 4}{4+4-2}\right)^3 \\ &\quad + 36(\chi-1)\left(\frac{4\times 8}{4+8-2}\right)^3 + 6(\chi-1)\left(\frac{8\times 8}{8+8-2}\right)^3 \\ &\quad + 48(\chi-1)\left(\frac{6\times 8}{6+8-2}\right)^3 \\ &\quad + 60(\chi-1)\left(\frac{6\times 6}{6+6-2}\right)^3 \\ &= 237.9177(\chi-1) + 176.65306 \\ &= 237.9177\chi - 61.26464. \end{aligned}$$

$$\begin{aligned} J(\Upsilon_1) &= \frac{192\chi+98}{(192\chi+98)-(72\chi-12)+2} \\ &\quad \times\left[\frac{48}{\sqrt{3\times 3}} + \frac{12(\chi-1)}{\sqrt{3\times 6}} + \frac{50+30(\chi-1)}{\sqrt{4\times 4}} + \frac{36(\chi-1)}{\sqrt{4\times 8}} + \frac{6(\chi-1)}{\sqrt{8\times 8}} + \frac{48(\chi-1)}{\sqrt{6\times 8}} + \frac{60(\chi-1)}{\sqrt{6\times 6}}\right] \\ &= \frac{192\chi+98}{120\chi+112}[34.37059(\chi-1)+28.5]. \end{aligned}$$

□

Theorem 3.7. *Let $\Upsilon_1 \cong L(MON_1(\chi))$ be a line graph of first metal–organic compound network with $\chi \geqslant 2$. Then the first, second and third redefine Zagreb indices are,*

$$\begin{aligned} 1 &: ReG_1(\Upsilon_1) = 70\chi - 13, \\ 2 &: ReG_2(\Upsilon_1) = 548.5714\chi - 376.5714, \\ 3 &: ReG_3(\Upsilon_1) = 83928\chi - 74936. \end{aligned}$$

Proof. Using concept in Eq. (19), value in Eq. (20) and formula from Eqs. (16)–(18), the results of first, second and third redefine Zagreb indices are computed as:

$$
\begin{aligned}
ReG_1(\Upsilon_1) = {} & \tfrac{3+3}{3\times3}(48) + 12(\chi-1)\tfrac{3+6}{3\times6} + (50+30(\chi-1))\tfrac{4+4}{4\times4} + 36(\chi-1)\tfrac{4+8}{4\times8} \\
& + 6(\chi-1)\tfrac{8+8}{8\times8} + 48(\chi-1)\tfrac{6+8}{6\times8} + 60(\chi-1)\tfrac{6+6}{6\times6} \\
= {} & 70(\chi-1) + 57 = 70\chi - 13 \\
ReG_2(\Upsilon_1) = {} & \tfrac{3\times3}{3+3}(48) + 12(\chi-1)\tfrac{3\times6}{3+6} + (50+30(\chi-1))\tfrac{4\times4}{4+4} + 36(\chi-1)\tfrac{4\times8}{4+8} \\
& + 6(\chi-1)\tfrac{8\times8}{8+8} + 48(\chi-1)\tfrac{6\times8}{6+8} + 60(\chi-1)\tfrac{6\times6}{6+6} \\
= {} & 548.5714(\chi-1) + 172 = 548.5714\chi - 376.5714 \\
ReG_3(\Upsilon_1) = {} & 3\times3\cdot(3+3)48 + 3\times6\cdot(3+6)(12(\chi-1)) + 4\times4\cdot(4+4)(50+30(\chi-1)) \\
& + 4\times8\cdot(4+8)(36(\chi-1)) + 8\times8\cdot(8+8)(6(\chi-1)) + 6\times8\cdot(6+8)(48(\chi-1)) \\
& + 6\times6\cdot(6+6)(60(\chi-1)) = 83928(\chi-1) + 8992 = 83928\chi - 74936
\end{aligned}
$$

□

4. Results of the Topological Indices of line graph of organic network $L(MON_2(\chi))$

In this section, we will discuss about line graph of second metal organic network $MON_2(\chi)$. The second metal organic network has also discussed in Hong et al. (2020) and line graph of second organic network $L(MON_2(2))$ as shown in Fig. 2. In this paper, we represents the line graph of second metal organic network $L(MON_2(\chi))$ as Υ_2. The order and size of $n_2 = V(\Upsilon_2) = 72\chi - 12$ and $m_2 = E(\Upsilon) = 156\chi + 102$ respectively. There are seven different types of edges in Υ_2 on the bases of different degree of end vertices. We have

$$
\begin{aligned}
E_1(3,3) &= \{ab \in E(\Upsilon_2(\chi)) | \zeta(a) = 3, \zeta(b) = 3\}, \\
E_2(3,4) &= \{ab \in E(\Upsilon_2(\chi)) | \zeta(a) = 3, \zeta(b) = 4\}, \\
E_3(4,4) &= \{ab \in E(\Upsilon_2(\chi)) | \zeta(a) = 4, \zeta(b) = 4\}, \\
E_4(4,5) &= \{ab \in E(\Upsilon_2(\chi)) | \zeta(a) = 4, \zeta(b) = 5\}, \\
E_5(5,5) &= \{ab \in E(\Upsilon_2(\chi)) | \zeta(a) = 5, \zeta(b) = 5\}, \\
E_6(5,6) &= \{ab \in E(\Upsilon_2(\chi)) | \zeta(a) = 5, \zeta(b) = 6\}, \\
E_7(6,6) &= \{ab \in E(\Upsilon_2(\chi)) | \zeta(a) = 6, \zeta(b) = 6\}, \\
E_8(6,6) &= \{ab \in E(\Upsilon_2(\chi)) | \zeta(a) = 6, \zeta(b) = 4\}.
\end{aligned}
\tag{21}
$$

where

$$
\begin{aligned}
|E(\Upsilon_2)| &= |E_1| + |E_2| + |E_3| + |E_4| + |E_5| + |E_6| + |E_7| + |E_8| = 48 + 12 + 36(\chi-1) \\
&\quad + 42 + 30(\chi-1) + 24(\chi-1) + 6(\chi-1) + 24(\chi-1) + 12(\chi-1) + 24(\chi-1) \\
&= 156\chi + 102.
\end{aligned}
\tag{22}
$$

Theorem 4.1. *Let $\Upsilon_2 \cong L(MON_2(\chi))$ be a line graph of second metal–organic compound network with $\chi \geqslant 2$. The general Randić indices are*

$$
\begin{aligned}
1: R_1(\Upsilon_2) &= 3270\chi - 2022, \\
2: R_{-1}(\Upsilon_2) &= 8.4483\chi + 0.5095, \\
3: R_{\frac{1}{2}}(\Upsilon_2) &= 703.06782\chi - 349.49862, \\
4: R_{-\frac{1}{2}}(\Upsilon_2) &= 35.73961799\chi - 5.7755.
\end{aligned}
$$

Proof. Using formula from Eqs. (1), (21) and (22), the general Randić indices are computed as below, when $\alpha = \pm1, \pm\frac{1}{2}$,

$$
\begin{aligned}
R_1(\Upsilon_2) = {} & 48(9) + (12+36(\chi-1))(12) + (42+30(\chi-1))(16) + 24(\chi-1)(20) \\
& + 6(\chi-1)(25) + 24(\chi-1)(30) + 12(\chi-1)(36) + 24(\chi-1)(24) \\
= {} & 3270(\chi-1) + 1248 = 3270\chi - 2022.
\end{aligned}
$$

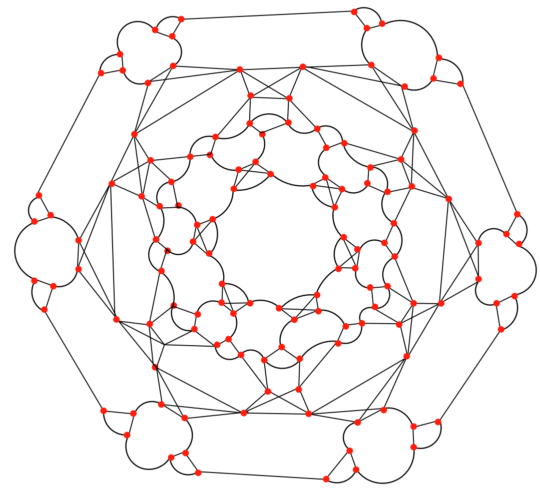

Fig. 2 Line grapph of metal–organic network $L(MON_1(2))$.

$$
\begin{aligned}
R_{-1}(\Upsilon_2) = {} & 48(9)^{-1} + (12+36(\chi-1))(12)^{-1} + (42+30(\chi-1))(16)^{-1} + 24(\chi-1)(20)^{-1} \\
& + 6(\chi-1)(25)^{-1} + 24(\chi-1)(30)^{-1} + 12(\chi-1)(36)^{-1} + 24(\chi-1)(24)^{-1} \\
= {} & 8.4483(\chi-1) + 8.95833 = 8.4483\chi + 0.5095. \\
R_{\frac{1}{2}}(\Upsilon_2) = {} & 48(9)^{\frac{1}{2}} + (12+36(\chi-1))(12)^{\frac{1}{2}} + (42+30(\chi-1))(16)^{\frac{1}{2}} + 24(\chi-1)(20)^{\frac{1}{2}} \\
& + 6(\chi-1)(25)^{\frac{1}{2}} + 24(\chi-1)(30)^{\frac{1}{2}} + 12(\chi-1)(36)^{\frac{1}{2}} + 24(\chi-1)(24)^{\frac{1}{2}} \\
= {} & 703.06782(\chi-1) + 353.5692 = 703.06782\chi - 349.49862. \\
R_{-\frac{1}{2}}(\Upsilon_2) = {} & 48(9)^{-\frac{1}{2}} + (12+36(\chi-1))(12)^{-\frac{1}{2}} + (42+30(\chi-1))(16)^{-\frac{1}{2}} + 24(\chi-1)(20)^{-\frac{1}{2}} \\
& + 6(\chi-1)(25)^{-\frac{1}{2}} + 24(\chi-1)(30)^{-\frac{1}{2}} + 12(\chi-1)(36)^{-\frac{1}{2}} + 24(\chi-1)(24)^{-\frac{1}{2}} \\
= {} & 35.73961799(\chi-1) + 29.96410 = 35.73961799\chi - 5.7755.
\end{aligned}
$$

□

Theorem 4.2. *Let $\Upsilon_2 \cong L(MON_2(\chi))$ be a line graph of second metal–organic compound network with $\chi \geqslant 2$. Then the atom bond connectivity and geometric arithmetic indices are*

$$
\begin{aligned}
1: ABC(\Upsilon_2) &= 80.52787\chi - 15.06237, \\
2: GA(\Upsilon_2) &= 144.897\chi - 43.0021.
\end{aligned}
$$

Proof. Using formula from Eqs. (2) and (3) along (21) and (22), the results are computed as:

$$
\begin{aligned}
ABC(\Upsilon_2) = {} & 48\sqrt{\tfrac{3+3-2}{3\times3}} + (12+36(\chi-1))\sqrt{\tfrac{3+4-2}{3\times4}} + (42+30(\chi-1))\sqrt{\tfrac{4+4-2}{4\times4}} \\
& + 24(\chi-1)\sqrt{\tfrac{4+5-2}{4\times5}} + 6(\chi-1)\sqrt{\tfrac{5+5-2}{5\times5}} + 24(\chi-1)\sqrt{\tfrac{5+6-2}{5\times6}} \\
& + 12(\chi-1)\sqrt{\tfrac{6+6-2}{6\times6}} + 24(\chi-1)\sqrt{\tfrac{6+4-2}{6\times4}} \\
= {} & 80.52787(\chi-1) + 65.4655 = 80.52787\chi - 15.06237.
\end{aligned}
$$

$$
\begin{aligned}
GA(\Upsilon_2) = {} & 48\tfrac{2\sqrt{3\times3}}{3+3} + (12+36(\chi-1))\tfrac{2\sqrt{3\times4}}{3+4} + (42+30(\chi-1))\tfrac{2\sqrt{4\times4}}{4+4} \\
& + 24(\chi-1)\tfrac{2\sqrt{4\times5}}{4+5} + 6(\chi-1)\tfrac{2\sqrt{5\times5}}{5+5} + 24(\chi-1)\tfrac{2\sqrt{5\times6}}{5+6} \\
& + 12(\chi-1)\tfrac{2\sqrt{6\times6}}{6+6} + 24(\chi-1)\tfrac{2\sqrt{6\times4}}{6+4} \\
= {} & 144.897(\chi-1) + 101.8769 = 144.897\chi - 43.0021.
\end{aligned}
$$

□

Theorem 4.3. *Let $\Upsilon_2 \cong L(MON_2(\chi))$ be a line graph of second metal–organic compound network with $\chi \geqslant 2$. Then the first, second Zagreb and hyper-Zagreb indices are*

$$\begin{aligned} 1: M_1(\Upsilon_2) &= 1416\chi - 708, \\ 2: M_2(\Upsilon_2) &= 3270\chi - 2022, \\ 3: HM(\Upsilon_2) &= 10840\chi - 5836. \end{aligned}$$

Proof. Putting Eqs. (21) and (22) in the formula from Eqs. (4), (5) and (6), the results computed as following:

$$\begin{aligned} M_1(\Upsilon_2) = {} & 48(3+3)+(12+36(\chi-1))(3+4)+(42+30(\chi-1))(4+4)+24(\chi-1)(4+5) \\ & + 6(\chi-1)(5+5)+24(\chi-1)(5+6)+12(\chi-1)(6+6)+24(\chi-1)(6+4) \\ & = 1416(\chi-1)+708 = 1416\chi-708. \\ M_2(\Upsilon_2) = {} & 48(3\times3)+(12+36(\chi-1))(3\times4)+(42+30(\chi-1))(4\times4)+24(\chi-1)(4\times5) \\ & + 6(\chi-1)(5\times5)+24(\chi-1)(5\times6)+12(\chi-1)(6\times6)+24(\chi-1)(6\times4) \\ & = 3270(\chi-1)+1248 = 3270\chi-2022. \\ HM(\Upsilon_2) = {} & 48(3+3)^2+(12+36(\chi-1))(3+4)^2+(42+30(\chi-1))(4+4)^2+24(\chi-1)(4+5)^2 \\ & + 6(\chi-1)(5+5)^2+24(\chi-1)(5+6)^2+12(\chi-1)(6+6)^2+24(\chi-1)(6+4)^2 \\ & = 10840(\chi-1)+5004 = 10840\chi-5836. \end{aligned}$$

□

Theorem 4.4. *Let $\Upsilon_2 \cong L(MON_2(\chi))$ be a line graph of second metal–organic compound network with $\chi \geqslant 2$. Then the first and second Zagreb coindices are*

$$\begin{aligned} 1: \overline{M_1}(\Upsilon_2) &= 22464\chi^2 + 9216\chi - 1944, \\ 2: \overline{M_2}(\Upsilon_2) &= 48672\chi^2 - 59670\chi + 23184. \end{aligned}$$

Proof. Putting Eqs. (21) and (22) in the formula from either Eqs. (7), (8) or Eqs. (9), (10), the results computed as following:

$$\begin{aligned} \overline{M_1}(\Upsilon_2) = {} & 2\cdot(156\chi+102)\cdot(72\chi-13)-(1416(\chi-1)+708) \\ & = 22464\chi^2+9216\chi-1944. \\ \overline{M_2}(\Upsilon_2) = {} & 2\cdot(156\chi+102)^2-\tfrac{1}{2}(1416(\chi-1)+708)-(3270(\chi-1)+1248) \\ & = 48672\chi^2-59670\chi+23184. \end{aligned}$$

□

Theorem 4.5. *Let $\Upsilon_2 \cong L(MON_2(\chi))$ be a line graph of second metal–organic compound network with $\chi \geqslant 2$. Then first and second multiplicative Zagreb indices are*

$$\begin{aligned} 1: PM_1(\Upsilon_2) &= 2^{144\chi+30}\cdot 3^{60\chi-12}\cdot 5^{30(\chi-1)}\cdot 7^{36\chi-24}\cdot 11^{24(\chi-1)}, \\ 2: PM_2(\Upsilon_2) &= 2^{360\chi-168}\cdot 3^{108\chi}\cdot 50^{60(\chi-1)}. \end{aligned}$$

Proof. Using formulae from Eqs. (11) and (12) along Eqs. (21) and (22), the first and second multiplicative Zagreb indices are computed as:

$$\begin{aligned} PM_1(\Upsilon_2) = {} & (3+3)^{48}\times(3+4)^{12+36(\chi-1)}\times(4+4)^{(42+30(\chi-1))}\times(4+5)^{24(\chi-1)} \\ & \times (5+5)^{6(\chi-1)}\times(5+6)^{24(\chi-1)}\times(6+6)^{12(\chi-1)}\times(6+4)^{24(\chi-1)} \\ & = 6^{48}\cdot 7^{12+36(\chi-1)}\cdot 8^{(42+30(\chi-1))}\cdot 9^{24(\chi-1)}\cdot 10^{6(\chi-1)}\cdot 11^{24(\chi-1)}\cdot 12^{12(\chi-1)}\cdot 10^{24(\chi-1)} \\ & = 2^{144\chi+30}\cdot 3^{60\chi-12}\cdot 5^{30(\chi-1)}\cdot 7^{36\chi-24}\cdot 11^{24(\chi-1)}. \\ PM_2(\Upsilon_2) = {} & (3\times3)^{48}\times(3\times4)^{12+36(\chi-1)}\times(4\times4)^{(42+30(\chi-1))}\times(4\times5)^{24(\chi-1)} \\ & \times (5\times5)^{6(\chi-1)}\times(5\times6)^{24(\chi-1)}\times(6\times6)^{12(\chi-1)}\times(6\times4)^{24(\chi-1)} \\ & = 9^{48}\cdot 12^{12+36(\chi-1)}\cdot 16^{42+30(\chi-1)}\cdot 20^{24(\chi-1)}\cdot 25^{6(\chi-1)}\cdot 30^{24(\chi-1)}\cdot 36^{12(\chi-1)}\cdot 24^{24(\chi-1)} \\ & = 2^{360\chi-168}\cdot 3^{108\chi}\cdot 50^{60(\chi-1)}. \end{aligned}$$

□

Theorem 4.6. *Let $\Upsilon_2 \cong L(MON_2(\chi))$ be a line graph of second metal–organic compound network with $\chi \geqslant 2$. Then the forgotten, augmented Zagreb and Balaban indices are*

$$\begin{aligned} 1: F(\Upsilon_2) &= 6720(\chi-1)+2508 = 6720\chi-4212, \\ 2: AZI(\Upsilon_2) &= 222.5384\chi - 37.0912, \\ 2: J(\Upsilon_2) &= \tfrac{156\chi+102}{84\chi+116}[35.7396(\chi-1)+29.964101]. \end{aligned}$$

Proof. Using formula from Eqs. (13), (14), (15), (21), and (22), the results computed as:

$$\begin{aligned} F(\Upsilon_2) = {} & 48(3^2+3^2)+(12+36(\chi-1))(3^2+4^2) \\ & +(42+30(\chi-1))(4^2+4^2)+24(\chi-1)(4^2+5^2) \\ & +6(\chi-1)(5^2+5^2)+24(\chi-1)(5^2+6^2)+12(\chi-1) \\ & \times(6^2+6^2)+24(\chi-1)(6^2+4^2) \\ = {} & 6720(\chi-1)+2508 = 6720\chi-4212. \end{aligned}$$

$$\begin{aligned} AZI(\Upsilon_2) = {} & 48\left(\frac{3\times3}{3+3-2}\right)^3+(12+36(\chi-1))\left(\frac{3\times4}{3+4-2}\right)^3 \\ & +(42+30(\chi-1))\left(\frac{4\times4}{4+4-2}\right)^3 \\ & +24(\chi-1)\left(\frac{4\times5}{4+5-2}\right)^3+6(\chi-1)\left(\frac{5\times5}{5+5-2}\right)^3 \\ & +24(\chi-1)\left(\frac{5\times6}{5+6-2}\right)^3 \\ & +12(\chi-1)\left(\frac{6\times6}{6+6-2}\right)^3 \\ & +24(\chi-1)\left(\frac{6\times4}{6+4-2}\right)^3 \\ = {} & 222.5384(\chi-1)+185.4472 \\ = {} & 222.5384\chi-37.0912. \end{aligned}$$

$$\begin{aligned} J(\Upsilon_2) = {} & \frac{156\chi+102}{(156\chi+102)-(72\chi-12)+2}\times\left[\frac{48}{\sqrt{3\times3}}+\frac{12+36(\chi-1)}{\sqrt{3\times4}}+\frac{42+30(\chi-1)}{\sqrt{4\times4}}+\frac{24(\chi-1)}{\sqrt{4\times5}}\right. \\ & \left.+\frac{6(\chi-1)}{\sqrt{5\times5}}+\frac{24(\chi-1)}{\sqrt{5\times6}}+\frac{12(\chi-1)}{\sqrt{6\times6}}+\frac{24(\chi-1)}{\sqrt{6\times4}}\right]=\frac{156\chi+102}{84\chi+116}[35.7396(\chi-1)+29.964101]. \end{aligned}$$

□

Theorem 4.7. *Let $\Upsilon_2 \cong L(MON_2(\chi))$ be a line graph of second metal–organic compound network with $\chi \geqslant 2$. The first, second and third redefine Zagreb indices are*

$$\begin{aligned} 1: ReG_1(\Upsilon_2) &= 67\chi - 7, \\ 2: ReG_2(\Upsilon_2) &= 349.1021\chi - 219.1974, \\ 3: ReG_3(\Upsilon_2) &= 31548\chi - 22572. \end{aligned}$$

Proof. Using formula from Eqs. (16), (17), (18), (22), ands (21), the results computed as:

$$\begin{aligned}
ReG_1(\Upsilon_2) = {} & \tfrac{3+3}{3\times 3}(48) + (12+36(\chi-1))\tfrac{3+4}{3\times 4} + (42+30(\chi-1))\tfrac{4+4}{4\times 4} + 24(\chi-1)\tfrac{4+5}{4\times 5} \\
& + 6(\chi-1)\tfrac{5+5}{5\times 5} + 24(\chi-1)\tfrac{5+6}{5\times 6} + 12(\chi-1)\tfrac{6+6}{6\times 6} + 12(\chi-1)\tfrac{6+4}{6\times 4} \\
= {} & 67(\chi-1) + 60 = 67\chi - 7. \\
ReG_2(\Upsilon_2) = {} & \tfrac{3\times 3}{3+3}(48) + (12+36(\chi-1))\tfrac{3\times 4}{3+4} + (42+30(\chi-1))\tfrac{4\times 4}{4+4} + 24(\chi-1)\tfrac{4\times 5}{4+5} \\
& + 6(\chi-1)\tfrac{5\times 5}{5+5} + 24(\chi-1)\tfrac{5\times 6}{5+6} + 12(\chi-1)\tfrac{6\times 6}{6+6} + 24(\chi-1)\tfrac{6\times 4}{6+4} \\
= {} & 349.1021(\chi-1) + 129.9047 = 349.1021\chi - 219.1974. \\
ReG_3(\Upsilon_2) = {} & 3\times 3\cdot(3+3)48 + 3\times 4\cdot(3+4)(12+36(\chi-1)) + 4\times 4\cdot(4+4)(42+30(\chi-1)) \\
& + 4\times 5\cdot(4+5)(24(\chi-1)) + 5\times 5\cdot(5+5)(6(\chi-1)) + 5\times 6\cdot(5+6)(24(\chi-1)) \\
& + 6\times 6\cdot(6+6)(12(\chi-1)) + 6\times 4\cdot(6+4)(24(\chi-1)) \\
= {} & 31548(\chi-1) + 8976 = 31548\chi - 22572.
\end{aligned}$$

□

5. Conclusion

In this paper, we discussed some physical properties of the line graph of the first and second metal–organic network in terms of topological indices, for this we computed different *TIs* such as Randić, atom bound connectivity, geometric arithmetic, Zagreb, Multiplicative Zagreb, and redefined Zagreb indices for line graph of first organic network $L(MON_1(\chi))$ and second organic network $L(MON_2(\chi)), \chi \geqslant 2$. We also computed the first and second Zagreb co-indices for the same networks. This computational work will help the researchers to understand the chosen structure more easily and will motivate the others to focus on the organic network. The computational method considered here are useful to analyse the physico-chemical properties of stated networks, and are cost effective and time efficient.

Author Contributions

All authors contributed equally for the preparation of this article.

Data Availability Statement

All data sets presented in this study are included in the article/Supplementary Material.

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Declaration of Competing Interest

The authors declare no conflict of interest.

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