

Research Article

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On computation of the reduced reverse degree and neighbourhood degree sum-based topological indices for metal-organic frameworks

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Abstract: Metal-organic frameworks (MOFs) are permeable substances with a high porosity volume, excellent chemical stability, and a distinctive shape created by strong interactions between metal ions and organic ligands. Work on the synthesis, structures, and properties of numerous MOFs demonstrates their usefulness in a variety of applications, including energy storage devices with good electrode materials, gas storage, heterogeneous catalysis, and chemical assessment. The physico-chemical characteristics of the chemical compounds in the underlying molecular graph or structure are predicted by a topological index, which is a numerical invariant. In this article, we look at two different metal-organic frameworks in terms of the number of layers, as well as metal and organic ligands. We compute the reduced reverse degree-based topological indices and some closed neighbourhood degree sum-based topological indices for these frameworks.

Keywords: reduced reverse degree, neighbourhood degree, topological indices, metal-organic frameworks

1 Introduction

Chemical reaction framework is a branch of applied mathematics aimed at replicating the behaviour of real-world chemical structures. Since its inception in the 19th century, it has grown in popularity among scientists, owing to advances in organic and theoretical chemistry.

Cheminformatics is a growing field in which quantitative structure-activity relationship and quantity structure-property relationship aid in the prediction of bioactivities and attributes of chemical compounds (Aslam et al., 2017; Ahmad et al., 2017; Doley et al., 2020). Physico-chemical characteristics and topological indices have been used to predict the bioactivity of organic molecules (Gutman, 2013).

The vertices in a chemical graph denote atoms or compounds, while the links depict the chemical bonding between them. Topological indices are numerical graph invariants that characterise the structure of the graph. The degree of a vertex is indicated by d_u or $d(u)$ (West, 2001) and it denotes the count of edges that are incident upon this vertex u .

Mondal et al. (2019) introduced some neighbourhood versions of degree-based indices such as Forgotten topological index F_N^* , second Zagreb index M_2^* , and hyper Zagreb index HM_N^* . Further, Mondal et al. (2021a) introduced six new neighbourhood degree sum indices, namely, ND_1 , ND_2 , ND_3 , ND_4 , ND_5 , and ND_6 . Many researchers are working on the QSPR analysis of various molecules (Al-Fahemi et al., 2014; Devillers and Balaban, 1999; Doley et al., 2020; Furtula and Gutman, 2015; Furtula et al., 2018; Hosamani, 2016, 2017; Mondal et al., 2021a,b), since it is an economically efficient mechanism to test compounds instead of testing them in a wet lab. Moreover, QSPR analysis can be used to develop models that can forecast properties or activities of organic chemical substances.

2 Preliminaries

Let G be a graph and v be a vertex of G . Kulli (2018) introduced the concept of reverse vertex degree $\mathcal{R}(v)$, defined as:

$$\mathcal{R}(v) = \Delta(G) - d(v) + 1 \quad (1)$$

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where $\Delta(G)$ is the maximum degree of the graph G and $d(v)$ is the degree of the vertex v .

Inspired by this definition, Ravi et al. (2021b) defined the reduced reverse degree as:

$$\mathcal{RR}(v) = \Delta(G) - d(v) + 2 \quad (2)$$

This was introduced to study the impact of the reduced reverse degree in the QSPR analysis. Further, they defined the reduced reverse degree-based versions of Zagreb indices, forgotten index, atom bond connectivity index, arithmetic index, and analysed their relationship with the physico-chemical properties of certain COVID-19 drugs.

The reduced reverse degree versions of the aforesaid topological indices are:

$$\text{RRM}_1(G) = \sum_{uv \in E} [\mathcal{RR}(u) + \mathcal{RR}(v)] \quad (3)$$

$$\text{RRM}_2(G) = \sum_{uv \in E} [\mathcal{RR}(u) * \mathcal{RR}(v)] \quad (4)$$

$$\text{RRHM}_1(G) = \sum_{uv \in E} [\mathcal{RR}(u) + \mathcal{RR}(v)]^2 \quad (5)$$

$$\text{RRHM}_2(G) = \sum_{uv \in E} [\mathcal{RR}(u) * \mathcal{RR}(v)]^2 \quad (6)$$

$$\text{RRF}(G) = \sum_{uv \in E} [\mathcal{RR}(u)^2 + \mathcal{RR}(v)^2] \quad (7)$$

$$\text{RRABC}(G) = \sum_{uv \in E} \left[\frac{\mathcal{RR}(u) + \mathcal{RR}(v) - 2}{\mathcal{RR}(u) * \mathcal{RR}(v)} \right] \quad (8)$$

$$\text{RRGA}(G) = \sum_{uv \in E} \left[\frac{2\sqrt{\mathcal{RR}(u) * \mathcal{RR}(v)}}{\mathcal{RR}(u) + \mathcal{RR}(v)} \right] \quad (9)$$

Ravi and co-authors proposed open (Ravi and Desikan, 2021a) and closed (Ravi and Desikan, 2022) neighbourhood degree sum-based topological indices. They computed those indices for the graphene structures and hyaluronic acid curcumin conjugates along with the QSPR analysis of octane isomers. The closed neighbourhood indices introduced by them are as follows:

$$\text{SK}_{N^c}(G) = \sum_{uv \in E(G)} \left[\frac{\delta_c[u] + \delta_c[v]}{2} \right] \quad (10)$$

$$\text{SK}_{1N^c}(G) = \sum_{uv \in E(G)} \left[\frac{\delta_c[u] * \delta_c[v]}{2} \right] \quad (11)$$

$$\text{SK}_{2N^c}(G) = \sum_{uv \in E(G)} \left[\frac{\delta_c[u] + \delta_c[v]}{2} \right]^2 \quad (12)$$

$$\text{mR}_{N^c}(G) = \sum_{uv \in E(G)} \left[\frac{1}{\max\{\delta_c[u], \delta_c[v]\}} \right] \quad (13)$$

$$\text{ISI}_{N^c}(G) = \sum_{uv \in E(G)} \left[\frac{\delta_c[u] * \delta_c[v]}{\delta_c[u] + \delta_c[v]} \right] \quad (14)$$

$$\text{RSK}_{N^c}(G) = \sum_{uv \in E(G)} \left[\frac{2}{\delta_c[u] + \delta_c[v]} \right] \quad (15)$$

$$\text{RSK}_{1N^c}(G) = \sum_{uv \in E(G)} \left[\frac{2}{\delta_c[u] * \delta_c[v]} \right] \quad (16)$$

$$\text{RSK}_{2N^c}(G) = \sum_{uv \in E(G)} \left[\frac{2}{\delta_c[u] + \delta_c[v]} \right]^2 \quad (17)$$

$$\text{RmR}_{N^c}(G) = \sum_{uv \in E(G)} [\max\{\delta_c[u], \delta_c[v]\}] \quad (18)$$

$$\text{RISI}_{N^c}(G) = \sum_{uv \in E(G)} \left[\frac{\delta_c[u] + \delta_c[v]}{\delta_c[u] * \delta_c[v]} \right] \quad (19)$$

where $\delta_c[u] = [\sum_{v \in N_G(u)} d(v)] + d(u)$, where $N_G(u)$ represents the open neighbourhood of the vertex u .

MOFs are used as catalysts in the preparation of numerous nanostructured materials (Yap et al., 2017). Wasson et al. (2008) gave the idea of linker competition within a metal-organic framework for structural insights. MOFs have crucial physical and chemical characteristics, such as changing organic ligands (Yin et al., 2015), transplanting (Hwang et al., 2008), post-synthetic ligand, and ion interchange (Kim et al., 2012), as well as impregnating appropriate effective materials (Thornton et al., 2009).

Various researchers (Agha et al., 2021, Ahmed and Jhung, 2014; Awais et al., 2020; Chu et al., 2020; Hong et al., 2020; Mumtaz et al., 2021; Xu et al., 2020; Zhao et al., 2021) have proposed different topological indices for the metal-organic frameworks.

In MOFs, the larger nodes correspond to zeolite imidazole (zinc-based metal), while the smaller nodes correspond to organic ligands. Between metals and organic ligands, as well between two organic ligands and two metals, the edges serve as connecting links. Now, we build two MOFs from the basic MOF by increasing the number of levels or dimensions that are made up of metals and organic ligands, with each new level or dimension adding two layers to the preceding level or dimension. For details on MOFs, refer Koo et al. (2017). The first metal-organic framework is created by forming links between the metals of two consecutive levels of the MOF, such that two metals in lower level are connected with a metal in the next level. Likewise, we create the second metal-organic framework by forming links among the organic ligands of two consecutive levels of the MOF, such that the two organic ligands in lower level are connected with an organic ligand in the next level.

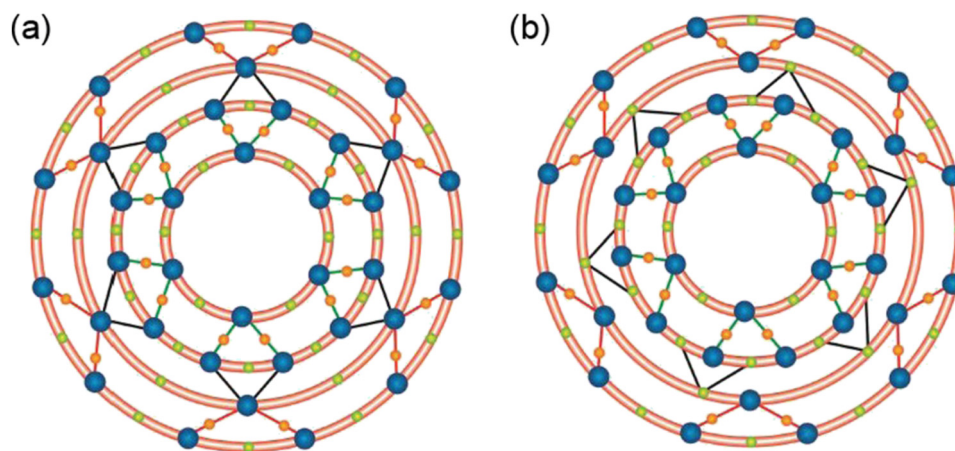


Figure 1: First (a) and second (b) metal-organic frameworks of dimension 2.

Furthermore, we have $|V(\text{MOF}_1(t))| = |V(\text{MOF}_2(t))| = 48t$ for both MOFs and $|E(\text{MOF}_1(t))| = |E(\text{MOF}_2(t))| = 72t - 12$ for both MO's. Figure 1 shows the first and second metal-organic framework ($\text{MOF}_1(t)$ and $\text{MOF}_2(t)$), for dimension $t = 2$. The figures of the first and second metal-organic frameworks are taken from the article by Awais et al. (2020).

3 Reduced reverse degree-based topological descriptors for the metal-organic frameworks

In this section, we compute the topological descriptors for both the metal-organic frameworks. We compute the reduced reverse degree-based versions of the Zagreb indices, forgotten index, atom bond connectivity index, and arithmetic index of the first and second metal-organic frameworks using the reduced reverse degree-based edge partitions.

Tables 1 and 2 provide the edge partitions of first and second metal-organic frameworks, respectively, based on the reduced reverse degrees of the end vertices.

Let $\text{MOF}_1(t)$ be the first metal-organic framework of dimension t , where $t \geq 2$.

Applying the reduced reverse degree-based edge partitions given in Table 1 in Eqs. 3–9, we get:

$$\begin{aligned} \text{RRM}_1(\text{MOF}_1(t)) &= \sum_{uv \in E} [\text{RR}(u) + \text{RR}(v)] \\ &= \sum_{uv \in E_1} [6 + 5] + \sum_{uv \in E_2} [6 + 4] + \sum_{uv \in E_3} [6 + 2] + \sum_{uv \in E_4} [4 + 2] \\ &= 624t + 12 \end{aligned}$$

$$\begin{aligned} \text{RRM}_2(\text{MOF}_1(t)) &= \sum_{uv \in E} [\text{RR}(u) * \text{RR}(v)] \\ &= \sum_{uv \in E_1} [6 * 5] + \sum_{uv \in E_2} [6 * 4] + \sum_{uv \in E_3} [6 * 2] + \sum_{uv \in E_4} [4 * 2] \\ &= 1,248t + 408 \end{aligned}$$

$$\begin{aligned} \text{RRHM}_1(\text{MOF}_1(t)) &= \sum_{uv \in E} [\text{RR}(u) + \text{RR}(v)]^2 \\ &= \sum_{uv \in E_1} [6 + 5]^2 + \sum_{uv \in E_2} [6 + 4]^2 \\ &\quad + \sum_{uv \in E_3} [6 + 2]^2 + \sum_{uv \in E_4} [4 + 2]^2 \\ &= 5,568t + 1,188 \end{aligned}$$

Table 1: Reduced degree edge partitions of $\text{MOF}_1(t)$

E_i	$(\text{RR}(u), \text{RR}(v))$	Count
E_1	(6, 5)	36
E_2	(6, 4)	$36t - 12$
E_3	(6, 2)	$24t - 24$
E_4	(4, 2)	$12t - 12$

Table 2: Reduced degree edge partitions of $\text{MOF}_2(t)$

E_i	$(\text{RR}(u), \text{RR}(v))$	Count
E_1	(4, 3)	$12t + 24$
E_2	(4, 2)	$12t + 12$
E_3	(3, 3)	$24t - 24$
E_4	(3, 2)	$12t - 12$
E_5	(2, 2)	$12t - 12$

$$\begin{aligned}
RRHM_2(MOF_1(t)) &= \sum_{uv \in E} [RR(u) * RR(v)]^2 \\
&= \sum_{uv \in E_1} [6 * 5]^2 + \sum_{uv \in E_2} [6 * 4]^2 + \sum_{uv \in E_3} [6 * 2]^2 + \sum_{uv \in E_4} [4 * 2]^2 \\
&= 24,960t + 21,265
\end{aligned}$$

$$\begin{aligned}
RRF(MOF_1(t)) &= \sum_{uv \in E} [RR(u)^2 + RR(v)^2] \\
&= \sum_{uv \in E_1} [6^2 + 5^2] + \sum_{uv \in E_2} [6^2 + 4^2] \\
&\quad + \sum_{uv \in E_3} [6^2 + 2^2] + \sum_{uv \in E_4} [4^2 + 2^2] \\
&= 3,072t + 372
\end{aligned}$$

$$\begin{aligned}
RRABC(MOF_1(t)) &= \sum_{uv \in E} \left[\sqrt{\frac{RR(u) + RR(v) - 2}{RR(u) * RR(v)}} \right] \\
&= \sum_{uv \in E_1} \left[\frac{6 + 5 - 2}{6 * 5} \right] + \sum_{uv \in E_2} \left[\frac{6 + 4 - 2}{6 * 4} \right] + \sum_{uv \in E_3} \left[\frac{6 + 2 - 2}{6 * 2} \right] + \sum_{uv \in E_4} \left[\frac{4 + 2 - 2}{4 * 2} \right] \\
&= 2 \left[\frac{9\sqrt{30} + 30\sqrt{3}t - 10\sqrt{3} + 45\sqrt{2}t - 45\sqrt{2}}{5} \right],
\end{aligned}$$

$$\begin{aligned}
RRGA(MOF_1(t)) &= \sum_{uv \in E} \left[\frac{2\sqrt{RR(u) * RR(v)}}{RR(u) + RR(v)} \right] \\
&= \sum_{uv \in E_1} \left[\frac{2\sqrt{6 * 5}}{6 + 5} \right] + \sum_{uv \in E_2} \left[\frac{2\sqrt{6 * 4}}{6 + 4} \right] + \sum_{uv \in E_3} \left[\frac{2\sqrt{6 * 2}}{6 + 2} \right] + \sum_{uv \in E_4} \left[\frac{2\sqrt{4 * 2}}{4 + 2} \right] \\
&= 4 \left[\frac{90\sqrt{30} + 198\sqrt{6}t - 66\sqrt{6} + 165\sqrt{3}t - 165\sqrt{3} + 110\sqrt{2}t - 110\sqrt{2}}{55} \right],
\end{aligned}$$

Let $MOF_2(t)$ be the second metal-organic framework of dimension t , for, $t \geq 2$.

Applying the reduced reverse degree-based edge partitions given in Table 2 in Eqs. 3–9, we get:

$$\begin{aligned}
RRM_1(MOF_2(t)) &= \sum_{uv \in E} [RR(u) + RR(v)] \\
&= \sum_{uv \in E_1} [4 + 3] + \sum_{uv \in E_2} [4 + 2] + \sum_{uv \in E_3} [3 + 3] \\
&\quad + \sum_{uv \in E_4} [3 + 2] + \sum_{uv \in E_5} [2 + 2] \\
&= 408t - 12
\end{aligned}$$

$$\begin{aligned}
RRM_2(MOF_2(t)) &= \sum_{uv \in E} [RR(u) * RR(v)] \\
&= \sum_{uv \in E_1} [4 * 3] + \sum_{uv \in E_2} [4 * 2] + \sum_{uv \in E_3} [3 * 3] \\
&\quad + \sum_{uv \in E_4} [3 * 2] + \sum_{uv \in E_5} [2 * 2] \\
&= 576t + 48
\end{aligned}$$

$$\begin{aligned}
RRHM_1(MOF_2(t)) &= \sum_{uv \in E} [RR(u) + RR(v)]^2 \\
&= \sum_{uv \in E_1} [4 + 3]^2 + \sum_{uv \in E_2} [4 + 2]^2 + \sum_{uv \in E_3} [3 + 3]^2 \\
&\quad + \sum_{uv \in E_4} [3 + 2]^2 + \sum_{uv \in E_5} [2 + 2]^2 \\
&= 2,376t + 252
\end{aligned}$$

$$\begin{aligned}
RRHM_2(MOF_2(t)) &= \sum_{uv \in E} [RR(u) * RR(v)]^2 \\
&= \sum_{uv \in E_1} [4 * 3]^2 + \sum_{uv \in E_2} [4 * 2]^2 + \sum_{uv \in E_3} [3 * 3]^2 \\
&\quad + \sum_{uv \in E_4} [3 * 2]^2 + \sum_{uv \in E_5} [2 * 2]^2 \\
&= 5,064t + 1,656
\end{aligned}$$

$$\begin{aligned}
RRF(MOF_2(t)) &= \sum_{uv \in E} [RR(u)^2 + RR(v)^2] \\
&= \sum_{uv \in E_1} [4^2 + 3^2] + \sum_{uv \in E_2} [4^2 + 2^2] + \sum_{uv \in E_3} [3^2 + 3^2] \\
&\quad + \sum_{uv \in E_4} [3^2 + 2^2] + \sum_{uv \in E_5} [2^2 + 2^2] \\
&= 1,224t + 156
\end{aligned}$$

$$\begin{aligned}
RRABC(MOF_2(t)) &= \sum_{uv \in E} \left[\sqrt{\frac{RR(u) + RR(v) - 2}{RR(u) * RR(v)}} \right] \\
&= \sum_{uv \in E_1} \left[\sqrt{\frac{4 + 3 - 2}{4 * 3}} \right] + \sum_{uv \in E_2} \left[\sqrt{\frac{4 + 2 - 2}{4 * 2}} \right] \\
&\quad + \sum_{uv \in E_3} \left[\sqrt{\frac{3 + 3 - 2}{3 * 3}} \right] \\
&\quad + \sum_{uv \in E_4} \left[\sqrt{\frac{3 + 2 - 2}{3 * 2}} \right] + \sum_{uv \in E_5} \left[\sqrt{\frac{2 + 2 - 2}{2 * 2}} \right] \\
&= 2[\sqrt{15}t + 2\sqrt{15} + 9t\sqrt{2} - 3\sqrt{2} + 8t - 8]
\end{aligned}$$

$$\begin{aligned}
\text{RRGA}(\text{MOF}_2(t)) &= \sum_{uv \in E} \left[\frac{2\sqrt{\text{RR}(u) * \text{RR}(v)}}{\text{RR}(u) + \text{RR}(v)} \right] \\
&= \sum_{uv \in E_1} \left[\frac{2\sqrt{4 * 3}}{4 + 3} \right] + \sum_{uv \in E_2} \left[\frac{2\sqrt{4 * 2}}{4 + 2} \right] + \sum_{uv \in E_3} \left[\frac{2\sqrt{3 * 3}}{3 + 3} \right] + \sum_{uv \in E_4} \left[\frac{2\sqrt{3 * 2}}{3 + 2} \right] + \sum_{uv \in E_5} \left[\frac{2\sqrt{2 * 2}}{2 + 2} \right] \\
&= 4 \left[\frac{60\sqrt{3}t + 120\sqrt{3} + 70\sqrt{2}t + 315t - 42\sqrt{6}t - 42\sqrt{6} - 315}{35} \right]
\end{aligned}$$

4 Neighbourhood degree sum-based topological descriptors for the metal-organic frameworks

In this section, we compute the neighbourhood degree sum based topological descriptors for both the metal-organic frameworks. We compute the topological indices

Table 3: Closed neighbourhood degree sum-based edge partitions of $\text{MOF}_1(t)$

E_i	(δ_u, δ_v)	Count
E_1	(8, 9)	24
E_2	(9, 11)	12
E_3	(10, 12)	23
E_4	(10, 16)	$24t - 12$
E_5	(11, 22)	12
E_6	(12, 16)	$12t - 24$
E_7	(12, 22)	$12t - 24$
E_8	(14, 22)	$12t - 12$
E_9	(16, 22)	$12t - 12$

Table 4: Closed neighbourhood degree sum-based edge partitions of $\text{MOF}_2(t)$

E_i	(δ_u, δ_v)	Count
E_1	(8, 9)	24
E_2	(9, 9)	12
E_3	(9, 11)	$12t - 12$
E_4	(9, 12)	12
E_5	(9, 16)	$12t - 12$
E_6	(10, 12)	12
E_7	(11, 13)	$24t - 24$
E_8	(13, 18)	$12t - 12$
E_9	(16, 18)	$12t - 12$

using the closed neighbourhood degree-sum of the end vertices. Tables 3 and 4 provide the edge partitions of first and second metal-organic frameworks based on the closed neighbourhood degree sum on the end vertices.

Let $\text{MOF}_1(t)$ be the first metal-organic framework of dimension t , for $t \geq 2$. Then, by applying the closed neighbourhood degree-sum edge partitions given in Table 3 in Eqs. 10–19, we get:

$$\begin{aligned}
\text{SK}_{N^c}(\text{MOF}_1(t)) &= |E_1| \left[\frac{8+9}{2} \right] + |E_2| \left[\frac{9+11}{2} \right] \\
&+ |E_3| \left[\frac{10+12}{2} \right] + |E_4| \left[\frac{10+16}{2} \right] + |E_5| \left[\frac{11+22}{2} \right] \\
&+ |E_6| \left[\frac{12+16}{2} \right] + |E_7| \left[\frac{12+22}{2} \right] + |E_8| \left[\frac{14+22}{2} \right] \\
&+ |E_9| \left[\frac{16+22}{2} \right] = 1,128t - 1,002
\end{aligned}$$

$$\begin{aligned}
\text{SK}_{1N^c}(\text{MOF}_1(t)) &= |E_1| \left[\frac{8*9}{2} \right] + |E_2| \left[\frac{9*11}{2} \right] \\
&+ |E_3| \left[\frac{10*12}{2} \right] + |E_4| \left[\frac{10*16}{2} \right] + |E_5| \left[\frac{11*22}{2} \right] \\
&+ |E_6| \left[\frac{12*16}{2} \right] + |E_7| \left[\frac{12*22}{2} \right] + |E_8| \left[\frac{14*22}{2} \right] \\
&+ |E_9| \left[\frac{16*22}{2} \right] = 8,616t - 10,002
\end{aligned}$$

$$\begin{aligned}
\text{SK}_{2N^c}(\text{MOF}_1(t)) &= |E_1| \left[\frac{8+9}{2} \right]^2 + |E_2| \left[\frac{9+11}{2} \right]^2 \\
&+ |E_3| \left[\frac{10+12}{2} \right]^2 + |E_4| \left[\frac{10+16}{2} \right]^2 + |E_5| \left[\frac{11+22}{2} \right]^2 \\
&+ |E_6| \left[\frac{12+16}{2} \right]^2 + |E_7| \left[\frac{12+22}{2} \right]^2 + |E_8| \left[\frac{14+22}{2} \right]^2 \\
&+ |E_9| \left[\frac{16+22}{2} \right]^2 = 18,096t - 21,003
\end{aligned}$$

$$\begin{aligned} \text{mR}_{N^c}(\text{MOF}_1(t)) &= |E_1| \left[\frac{1}{9} \right] + |E_2| \left[\frac{1}{11} \right] \\ &+ |E_3| \left[\frac{1}{12} \right] + |E_4| \left[\frac{1}{16} \right] + |E_5| \left[\frac{1}{22} \right] + |E_6| \left[\frac{1}{16} \right] \\ &+ |E_7| \left[\frac{1}{22} \right] + |E_8| \left[\frac{1}{22} \right] + |E_9| \left[\frac{1}{22} \right] \\ &= \frac{513t + 103}{132} \end{aligned}$$

$$\begin{aligned} \text{ISI}_N(\text{MOF}_1(t)) &= |E_1| \left[\frac{8 \cdot 9}{8 + 9} \right] \\ &+ |E_2| \left[\frac{9 \cdot 11}{9 + 11} \right] + |E_3| \left[\frac{10 \cdot 12}{10 + 12} \right] + |E_4| \left[\frac{10 \cdot 16}{10 + 16} \right] \\ &+ |E_5| \left[\frac{11 \cdot 22}{11 + 22} \right] + |E_6| \left[\frac{12 \cdot 16}{12 + 16} \right] + |E_7| \left[\frac{12 \cdot 22}{12 + 22} \right] \\ &+ |E_8| \left[\frac{14 \cdot 22}{14 + 22} \right] + |E_9| \left[\frac{16 \cdot 22}{16 + 22} \right] \\ &= 536.9791t - 472.4635 \end{aligned}$$

$$\begin{aligned} \text{RSK}_{N^c}(\text{MOF}_1(t)) &= |E_1| \left[\frac{2}{8 + 9} \right] + |E_2| \left[\frac{2}{9 + 11} \right] \\ &+ |E_3| \left[\frac{2}{10 + 12} \right] + |E_4| \left[\frac{2}{10 + 16} \right] + |E_5| \left[\frac{2}{11 + 22} \right] \\ &+ |E_6| \left[\frac{2}{12 + 16} \right] + |E_7| \left[\frac{2}{12 + 22} \right] + |E_8| \left[\frac{2}{14 + 22} \right] \\ &+ |E_9| \left[\frac{2}{16 + 22} \right] \\ &= 4.7074t + 0.2870 \end{aligned}$$

$$\begin{aligned} \text{RSK1}_{N^c}(\text{MOF}_1(t)) &= |E_1| \left[\frac{2}{8 \cdot 9} \right] + |E_2| \left[\frac{2}{9 \cdot 11} \right] \\ &+ |E_3| \left[\frac{2}{10 \cdot 12} \right] + |E_4| \left[\frac{2}{10 \cdot 16} \right] + |E_5| \left[\frac{2}{11 \cdot 22} \right] \\ &+ |E_6| \left[\frac{2}{12 \cdot 16} \right] + |E_7| \left[\frac{2}{12 \cdot 22} \right] + |E_8| \left[\frac{2}{14 \cdot 22} \right] \\ &+ |E_9| \left[\frac{2}{16 \cdot 22} \right] = 0.6620t + 0.5342 \end{aligned}$$

$$\begin{aligned} \text{RSK2}_{N^c}(\text{MOF}_1(t)) &= |E_1| \left[\frac{2}{8 + 9} \right]^2 + |E_2| \left[\frac{2}{9 + 11} \right]^2 \\ &+ |E_3| \left[\frac{2}{10 + 12} \right]^2 + |E_4| \left[\frac{2}{10 + 16} \right]^2 + |E_5| \left[\frac{2}{11 + 22} \right]^2 \\ &+ |E_6| \left[\frac{2}{12 + 16} \right]^2 + |E_7| \left[\frac{2}{12 + 22} \right]^2 + |E_8| \left[\frac{2}{14 + 22} \right]^2 \\ &+ |E_9| \left[\frac{2}{16 + 22} \right]^2 \\ &= 0.3150t + 0.2775 \end{aligned}$$

$$\begin{aligned} \text{RmR}_{N^c}(\text{MOF}_1(t)) &= |E_1| [9] + |E_2| [11] + |E_3| [12] \\ &+ |E_4| [16] + |E_5| [22] + |E_6| [16] + |E_7| [22] \\ &+ |E_8| [22] + |E_9| [22] \\ &= 1,368t - 1,260 \end{aligned}$$

$$\begin{aligned} \text{RISI}_{N^c}(\text{MOF}_1(t)) &= |E_1| \left[\frac{8 + 9}{8 \cdot 9} \right] + |E_2| \left[\frac{9 + 11}{9 \cdot 11} \right] \\ &+ |E_3| \left[\frac{10 + 12}{10 \cdot 12} \right] + |E_4| \left[\frac{10 + 16}{10 \cdot 16} \right] + |E_5| \left[\frac{11 + 22}{11 \cdot 22} \right] \\ &+ |E_6| \left[\frac{12 + 16}{12 \cdot 16} \right] + |E_7| \left[\frac{12 + 22}{12 \cdot 22} \right] + |E_8| \left[\frac{14 + 22}{14 \cdot 22} \right] \\ &+ |E_9| \left[\frac{16 + 22}{16 \cdot 22} \right] \\ &= 9.8935t + 0.1903 \end{aligned}$$

Let $\text{MOF}_2(t)$ be the second metal-organic framework of dimension t , for $t \geq 2$. Then, by applying the closed neighbourhood degree-sum edge partitions given in Table 4 in Eqs. 10–19, we get:

$$\begin{aligned} \text{SK}_{N^c}(\text{MOF}_2(t)) &= |E_1| \left[\frac{8+9}{2} \right] + |E_2| \left[\frac{9+9}{2} \right] \\ &+ |E_3| \left[\frac{9+11}{2} \right] + |E_4| \left[\frac{9+12}{2} \right] + |E_5| \left[\frac{9+16}{2} \right] \\ &+ |E_6| \left[\frac{10+12}{2} \right] + |E_7| \left[\frac{11+13}{2} \right] + |E_8| \left[\frac{13+18}{2} \right] \\ &+ |E_9| \left[\frac{16+18}{2} \right] \\ &= 948t + 172 \end{aligned}$$

$$\begin{aligned} \text{SK1}_{N^c}(\text{MOF}_2(t)) &= |E_1| \left[\frac{8 \cdot 9}{2} \right] + |E_2| \left[\frac{9 \cdot 9}{2} \right] \\ &+ |E_3| \left[\frac{9 \cdot 11}{2} \right] + |E_4| \left[\frac{9 \cdot 12}{2} \right] + |E_5| \left[\frac{9 \cdot 16}{2} \right] \\ &+ |E_6| \left[\frac{10 \cdot 12}{2} \right] + |E_7| \left[\frac{11 \cdot 13}{2} \right] + |E_8| \left[\frac{13 \cdot 18}{2} \right] \\ &+ |E_9| \left[\frac{16 \cdot 18}{2} \right] \\ &= 6,306t + 237 \end{aligned}$$

$$\begin{aligned} \text{SK2}_{N^c}(\text{MOF}_2(t)) &= |E_1| \left[\frac{8 + 9}{2} \right]^2 + |E_2| \left[\frac{9 + 9}{2} \right]^2 \\ &+ |E_3| \left[\frac{9 + 11}{2} \right]^2 + |E_4| \left[\frac{9 + 12}{2} \right]^2 + |E_5| \left[\frac{9 + 16}{2} \right]^2 \\ &+ |E_6| \left[\frac{10 + 12}{2} \right]^2 + |E_7| \left[\frac{11 + 13}{2} \right]^2 + |E_8| \left[\frac{13 + 18}{2} \right]^2 \\ &+ |E_9| \left[\frac{16 + 18}{2} \right]^2 \\ &= 12,882t + 454 \end{aligned}$$

$$\begin{aligned} \text{mR}_{N^c}(\text{MOF}_2(t)) &= |E_1| \left[\frac{1}{9} \right] + |E_2| \left[\frac{1}{9} \right] + |E_3| \left[\frac{1}{11} \right] \\ &+ |E_4| \left[\frac{1}{12} \right] + |E_5| \left[\frac{1}{16} \right] + |E_6| \left[\frac{1}{12} \right] + |E_7| \left[\frac{1}{13} \right] \\ &+ |E_8| \left[\frac{1}{18} \right] + |E_9| \left[\frac{1}{18} \right] \\ &= \frac{51,690t + 37,321}{10,296} \end{aligned}$$

$$\begin{aligned} \text{ISI}_{N^c}(\text{MOF}_2(t)) &= |E_1| \left[\frac{8 \cdot 9}{8+9} \right] + |E_2| \left[\frac{9 \cdot 9}{9+9} \right] \\ &+ |E_3| \left[\frac{9 \cdot 11}{9+11} \right] + |E_4| \left[\frac{9 \cdot 12}{9+12} \right] + |E_5| \left[\frac{9 \cdot 16}{9+16} \right] \\ &+ |E_6| \left[\frac{10 \cdot 12}{10+12} \right] + |E_7| \left[\frac{11 \cdot 13}{11+13} \right] + |E_8| \left[\frac{13 \cdot 18}{13+18} \right] \\ &+ |E_9| \left[\frac{16 \cdot 18}{16+18} \right] \\ &= 463.7477t + 86.3579 \end{aligned}$$

$$\begin{aligned} \text{RSK}_{N^c}(\text{MOF}_2(t)) &= |E_1| \left[\frac{2}{8+9} \right] + |E_2| \left[\frac{2}{9+9} \right] \\ &+ |E_3| \left[\frac{2}{9+11} \right] + |E_4| \left[\frac{2}{9+12} \right] + |E_5| \left[\frac{2}{9+16} \right] \\ &+ |E_6| \left[\frac{2}{10+12} \right] + |E_7| \left[\frac{2}{11+13} \right] + |E_8| \left[\frac{2}{13+18} \right] \\ &+ |E_9| \left[\frac{2}{16+18} \right] \\ &= 5.6401t + 3.7839 \end{aligned}$$

$$\begin{aligned} \text{RSK1}_{N^c}(\text{MOF}_2(t)) &= |E_1| \left[\frac{2}{8 \cdot 9} \right] + |E_2| \left[\frac{2}{9 \cdot 9} \right] \\ &+ |E_3| \left[\frac{2}{9 \cdot 11} \right] + |E_4| \left[\frac{2}{9 \cdot 12} \right] + |E_5| \left[\frac{2}{9 \cdot 16} \right] \\ &+ |E_6| \left[\frac{2}{10 \cdot 12} \right] + |E_7| \left[\frac{2}{11 \cdot 13} \right] + |E_8| \left[\frac{2}{13 \cdot 18} \right] \\ &+ |E_9| \left[\frac{2}{16 \cdot 18} \right] \\ &= 0.9307t + 0.9504 \end{aligned}$$

$$\begin{aligned} \text{RSK2}_{N^c}(\text{MOF}_2(t)) &= |E_1| \left[\frac{2}{8+9} \right]^2 + |E_2| \left[\frac{2}{9+9} \right]^2 \\ &+ |E_3| \left[\frac{2}{9+11} \right]^2 + |E_4| \left[\frac{2}{9+12} \right]^2 + |E_5| \left[\frac{2}{9+16} \right]^2 \\ &+ |E_6| \left[\frac{2}{10+12} \right]^2 + |E_7| \left[\frac{2}{11+13} \right]^2 + |E_8| \left[\frac{2}{13+18} \right]^2 \\ &+ |E_9| \left[\frac{2}{16+18} \right]^2 = 0.4549t + 0.4736 \end{aligned}$$

$$\begin{aligned} \text{RmR}_{N^c}(\text{MOF}_2(t)) &= |E_1|[9] + |E_2|[9] + |E_3|[11] \\ &+ |E_4|[12] + |E_5|[16] + |E_6|[12] + |E_7|[13] \\ &+ |E_8|[18] + |E_9|[18] = 1,068t + 174 \end{aligned}$$

$$\begin{aligned} \text{RISI}_{N^c}(\text{MOF}_2(t)) &= |E_1| \left[\frac{8+9}{8 \cdot 9} \right] + |E_2| \left[\frac{9+9}{9 \cdot 9} \right] \\ &+ |E_3| \left[\frac{9+11}{9 \cdot 11} \right] + |E_4| \left[\frac{9+12}{9 \cdot 12} \right] + |E_5| \left[\frac{9+16}{9 \cdot 16} \right] \\ &+ |E_6| \left[\frac{10+12}{10 \cdot 12} \right] + |E_7| \left[\frac{11+13}{11 \cdot 13} \right] + |E_8| \left[\frac{13+18}{13 \cdot 18} \right] \\ &+ |E_9| \left[\frac{16+18}{16 \cdot 18} \right] = 11.5420t + 7.5864 \end{aligned}$$

5 Conclusion

Computing various topological indices of chemical graphs allows for the investigation of chemical molecules and research of how the indices connect to the physiochemical properties. In this article, we determined the cardinality of the reduced reverse degree-based and closed neighbourhood degree-sum edge partitions corresponding to two metal-organic frameworks, $\text{MOF}_1(t)$ and $\text{MOF}_2(t)$, respectively. These edge partitions were used to compute the reduced reverse degree-based topological indices and some closed neighbourhood degree sum-based topological indices for $\text{MO}_1(t)$ and $\text{MO}_2(t)$, respectively. As future work, we plan to apply these descriptors to various transformations of metal-organic frameworks and to analyse the physico-chemical properties of the metal-organic frameworks like electrochemical stability and flexibility.

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