

Research Article

Computation of Vertex-Based Topological Descriptors of Organometallic Monolayers of $TM_3C_{12}S_{12}$

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Topological descriptors are mathematical values related to chemical structures which are associated with different physico-chemical properties. The use of topological descriptors has a great contribution in the field of quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) modeling. These are mathematical relationships between different molecular properties or biological activity and some other physicochemical or structural properties. In this article, we calculate few vertex degree-based topological indices/descriptors of the organometallic monolayer structure. At present, the numerical programming of the biological structure with topological descriptors is increasing in consequence in invigorating science, bioinformatics, and pharmaceuticals.

1. Introduction

Metal-organic structures (MOs) are presented by the three-dimensional systems that are produced by the connections of natural linkers and metal center atoms. In the MOs, natural linkers associate all metal center atoms to develop networks that can contain a scope of visitor particles. This class of material get consideration by more objective ways to deal with their reticular plan and amalgamation. Moreover, there have been tens of thousands of metal-organic frameworks inserted. It extends the degree of their probable applications. These MOs have been found to be useful in the field of gas catalysis [1–3], drugs' conveyance [4–6], detection [7, 8], separations [9, 10], storage [11–13], and adsorption [14–18]. These structures have a lot of open metal terminals that can catch industrial exhaust gases such as NO, CO, NO₂, CO₂, and SO₂. The discharge of CO₂ from flue gases has a negative impact on the environment from consuming of nonsustainable power sources which is a

critical issue for the ecological change and greenhouse effect. Gases such as SO₂ and NO₂ are primary justification acceptance of corrosive downpour just as smog, while NO and CO are dangerous for us. In this way, to have a sound air, controlling the entrance of these dangerous gases into the atmosphere is necessary. They may be able to capture CO₂ from the flue gases of power plants. At room temperature and with a low pressing factor, MOs-74 can capture CO₂. More information on the ability of metal-organic frameworks to trap pipe gas particles can be found in [19, 20].

2. Preliminaries

A molecular graph represents the structural formula of a chemical molecule. The atoms are denoted by the vertices, whereas the bonds between the vertices are denoted by the edges. Assume $G(V(G), E(G))$ is a molecular graph, with the vertex and edge sets $V(G)$ and $E(G)$, respectively. They

are together if two vertices z and r are end vertices of a shared edge $e = zr$. N_z represents the collection of neighbors of a vertex z and is defined as $N_z = \{r \in V(G) : zr \in E(G)\}$. The cardinality of the set N_z is represented by the degree of a vertex z , which is represented by d_z . $S_z = \sum_{r \in N_z} d_r$, S_z explains the sum of degrees of neighbors of z .

In 1975, the primary degree-based topological descriptor was presented by Milan Randić [21]. Randić index is denoted by $R_{-1/2}(G)$. It is characterized as follows:

$$R_{-1/2}(G) = \sum_{st \in E(G)} \frac{1}{\sqrt{d_s d_t}} \quad (1)$$

The first and second Zagreb indices, which are beneficial for branching questions, were proposed by Gutman [22] in 1972. These are represented by the variables $M_1(G)$ and $M_2(G)$, which are defined as follows:

$$\begin{aligned} M_1(G) &= \sum_{st \in E(G)} (d_s + d_t), \\ M_2(G) &= \sum_{st \in E(G)} (d_s \times d_t). \end{aligned} \quad (2)$$

The Zagreb indices and their variants have been employed to study subatomic intricacy [23, 24], chirality, ZE-isomerism, and heterosystems, and the general Zagreb indices have a reasonable relevance for inferring multilinear relapse models. The Zagreb indices are used by a number of analysts in their QSPR and QSAR investigations. The sum-connectivity index is also a highly valuable index. It is closely linked to hydrocarbons' π electron energy. It is defined as follows:

$$SCI(G) = \sum_{st \in E(G)} \frac{1}{\sqrt{d_s + d_t}} \quad (3)$$

Currently, Zhou and Trinajstić [25] have proposed the general sum-connectivity index. It has the following definition:

$$\chi_\alpha(G) = \sum_{st \in E(G)} (d_s + d_t)^\alpha \quad (4)$$

Recently, hyper-Zagreb index was introduced by Shirdel et al. [26]. It is defined as

$$HM(G) = \sum_{st \in E(G)} [d_s + d_t]^2 \quad (5)$$

Estrada et al. [27] presented the atom-bond connectivity (ABC) index in 1998. It is defined as follows:

$$ABC(G) = \sum_{st \in E(G)} \sqrt{\frac{d_s + d_t - 2}{d_s d_t}} \quad (6)$$

It presents a better representation for adjusting direct and spread alkanes. Moreover, the energy is stored in cycloalkanes due to the deformation of cycloalkanes. A very common connectivity index is known as the geometric-arithmetic (GA) index which was discussed by Xiao et al. in [28]. For any graph G , the geometric-arithmetic index (GA) is denoted and defined as follows:

$$GA(G) = \sum_{st \in E(G)} \frac{2\sqrt{d_s d_t}}{d_s + d_t} \quad (7)$$

In the case of octane isomers, it has been presented that the GA index has good relationships with a range of different physicochemical properties [29, 30].

3. Computational Aspects

In this section, the two-dimensional organometallic monolayers of the $TM_3C_{12}S_{12}$ coordination network will be discussed. The $TM_3C_{12}S_{12}$ metal-organic framework is a kind of very important chemical structure for the purpose of its significant application in the field of drug industry. In the recent times, the researchers and scientists have begun to pay more attention to the catalytic performance of the organometallic structures which are the combination of some kinds of transition metal and organic structures. The metals which can be used in the place of TM_3 are ($M = Fe, Co, Ni, Ru, Rh, Pd, Os, Ir, \text{ and } Pt$). Now, the basic purpose of our work is to provide basic and necessary mathematical values in the form of topological indices to the researchers and scientists which can help them in enlarging the physical and chemical properties of metal-organic frameworks.

Figure 1 shows the schematic geometric structure of the $TM_3C_{12}S_{12}$ monolayer; (a) and (f) are top views of one unit cell and 2×2 supercells, respectively. Only (b), (d), and (e) are visible after structural optimization, as shown in side views of four alternative beginning configurations. The C, S, and TM atoms of the first transition metal are represented by the black, yellow, and purple balls, respectively. The molecular graph of a 2D metal-organic supercell with g unit cells in each row and h unit cells in each column is $\mathcal{G}_2(g, h)$. The graph $\mathcal{G}_{2(2,2)}$ is shown in Figure 1. A quick look at the graph $\mathcal{G}_2(g, h)$ reveals that it has $36gh$ vertices and $36gh + 2g + 2h$ edges.

The general Randić index and general sum-connectivity index of $\mathcal{G}_2(g, h)$ are computed in the next theorem.

Theorem 1. *The Randić and general sum-connectivity indices of the graph $\mathcal{G}_2(g, h)$ are as follows:*

$$\begin{aligned} R_\alpha(\mathcal{G}_2(g, h)) &= (4g + 4h)(4)^\alpha + (12gh)(6)^\alpha \\ &\quad + (12gh - 4g - 4h)(8)^\alpha + (12gh)(9)^\alpha, \\ \chi_\alpha(\mathcal{G}_2(g, h)) &= (4g + 4h)(4)^\alpha + (12gh)(5)^\alpha \\ &\quad + (12gh - 4g - 4h)(6)^\alpha + (12gh)(6)^\alpha. \end{aligned} \quad (8)$$

Proof. The edge partition of the graph $\mathcal{G}_2(g, h)$ will be obtained first in order to measure the general Randić and general sum-connectivity indices. The degree of the end vertex is needed in this regard. In Table 1, the partition is mentioned.

Similarly, in the definitions of the aforementioned indices, the values of the edge partition are used. The computation of the Randić index is as follows:

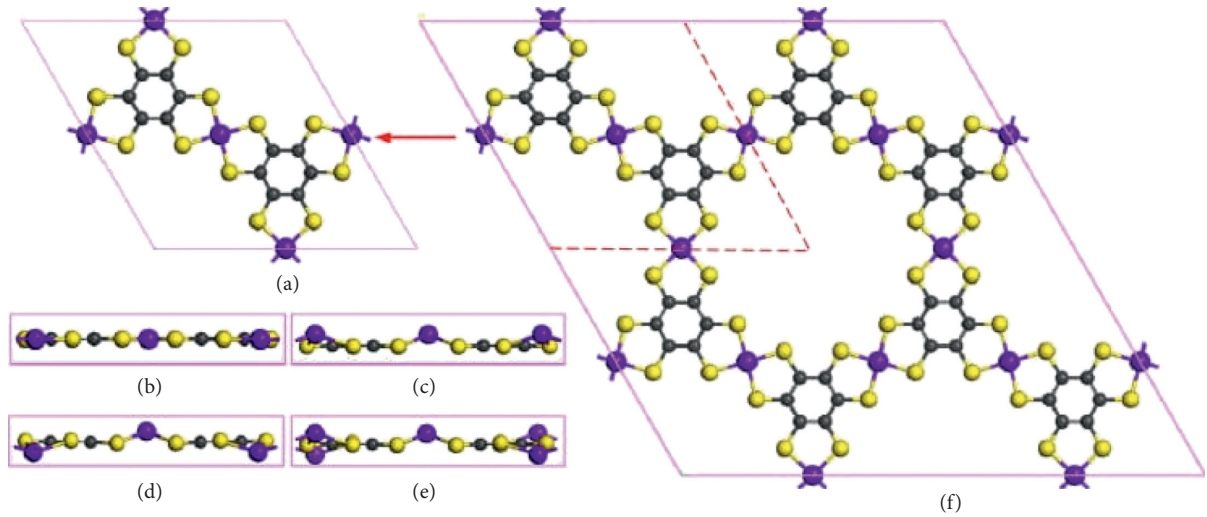


FIGURE 1: Schematic geometric structure of the (2×2) supercell of organometallic monolayers of $\text{TM}_3\text{C}_{12}\text{S}_{12}$; the unit cell is represented within the box.

TABLE 1: The edge partition of graph $\mathcal{G}_2(g, h)$ based on degrees of end vertices of each edge.

(d_s, d_t) where $st \in E(\mathcal{G}_2(g, h))$	Number of edges
$(2, 2)$	$4g + 4h$
$(2, 3)$	$12gh$
$(2, 4)$	$12gh - 4g - 4h$
$(3, 3)$	$12gh$

$$\begin{aligned}
 R_\alpha(\mathcal{G}_2(g, h)) &= \sum_{st \in E_{(2,2)}(\mathcal{G}_2(g, h))} (d_s d_t)^\alpha + \sum_{st \in E_{(2,3)}(\mathcal{G}_2(g, h))} (d_s d_t)^\alpha + \sum_{st \in E_{(2,4)}(\mathcal{G}_2(g, h))} (d_s d_t)^\alpha + \sum_{st \in E_{(3,3)}(\mathcal{G}_2(g, h))} (d_s d_t)^\alpha, \\
 &= (4g + 4h)(2 \times 2)^\alpha + (12gh)(2 \times 3)^\alpha + (12gh - 4g - 4h)(2 \times 4)^\alpha + (12gh)(3 \times 3)^\alpha \\
 &= (4g + 4h)(4)^\alpha + (12gh)(6)^\alpha + (12gh - 4g - 4h)(8)^\alpha + (12gh)(9)^\alpha, \\
 \chi_\alpha(\mathcal{G}_2(g, h)) &= \sum_{st \in \mathcal{E}_{(2,2)}(\mathcal{G}_2(g, h))} (d_s + d_t)^\alpha + \sum_{st \in \mathcal{E}_{(2,3)}(\mathcal{G}_2(g, h))} (d_s + d_t)^\alpha + \sum_{st \in \mathcal{E}_{(2,4)}(\mathcal{G}_2(g, h))} (d_s + d_t)^\alpha + \sum_{st \in \mathcal{E}_{(3,3)}(\mathcal{G}_2(g, h))} (d_s + d_t)^\alpha, \\
 &= (4g + 4h)(2 + 2)^\alpha + (12gh)(2 + 3)^\alpha + (12gh - 4g - 4h)(2 + 4)^\alpha + (12gh)(3 + 3)^\alpha \\
 &= (4g + 4h)(4)^\alpha + (12gh)(5)^\alpha + (12gh - 4g - 4h)(6)^\alpha + (12gh)(6)^\alpha.
 \end{aligned} \tag{9}$$

Corollary 1. Using Theorem 1, with values of $\alpha = -1/2, 1,$ and -1 , the Randic connectivity index, the first Zagreb index, the second Zagreb index, and the sum-connectivity index can be calculated as follows:

$$\begin{aligned}
 R_{-1/2}(\mathcal{G}_2(g, h)) &= \frac{4547}{346}gh + \frac{577}{985}g + \frac{577}{985}h, \\
 M_1(\mathcal{G}_2(g, h)) &= 204gh - 8g - 8h, \\
 M_2(\mathcal{G}_2(g, h)) &= 276gh - 16g - 16h, \\
 \text{SCI}(\mathcal{G}_2(g, h)) &= \frac{5899}{389}gh + \frac{396}{1079}g + \frac{396}{1079}b, \\
 \text{HM}(\mathcal{G}_2(g, h)) &= 1164gh - 80g - 80h.
 \end{aligned} \tag{10}$$

In the next theorem, the atom-bond connectivity index and geometric-arithmetic index of the graph $\mathcal{G}_2(g, h)$ are calculated.

Theorem 2. The atom-bond connectivity (ABC) index and geometric-arithmetic (GA) index of the graph $\mathcal{G}_2(g, h)$ are as follows:

$$\begin{aligned}
 \text{ABC}(\mathcal{G}_2(g, h)) &= \frac{985}{1393}gh + \frac{985}{1393}g + \frac{2}{3}b, \\
 \text{GA}(\mathcal{G}_2(g, h)) &= \frac{14765}{421}gh - \frac{272}{1189}g - \frac{272}{1189}h.
 \end{aligned} \tag{11}$$

Proof. In the description of the atom-bond connectivity index, different values of the edge partition are used. It can be calculated in the following manner:

$$\begin{aligned}
ABC(\mathcal{G}_2(g, h)) &= (4g + 4h)\left(\frac{985}{1393}\right) + (12gh)\left(\frac{985}{1393}\right) \\
&\quad + (12gh - 4g - 4h)\left(\frac{985}{1393}\right) + (12gh)\left(\frac{2}{3}\right), \\
&= \frac{28841}{1155}gh + 0g + 0h.
\end{aligned} \tag{12}$$

Similarly, the geometric-arithmetic (GA) index can be calculated as follows:

$$\begin{aligned}
GA(\mathcal{G}_2(g, h)) &= (4g + 4h)(1) + (12gh)\left(\frac{4704}{4801}\right) \\
&\quad + (12gh - 4g - 4h)\left(\frac{1121}{1189}\right) + (12gh)(1). \\
&= \frac{14765}{421}gh - \frac{272}{1189}g - \frac{272}{1189}h.
\end{aligned} \tag{13}$$

Moreover, in the following theorem, the fourth version of the atom-bond connectivity (ABC_4) index and the fifth version of the geometric-arithmetic (GA_5) index are obtained.

Theorem 3. *The fourth type of atom-bond connectivity index (ABC_4) and fifth type of geometric-arithmetic index (GA_5) of the given graph $\mathcal{G}_2(g, h)$ are as follows:*

$$\begin{aligned}
ABC_4(\mathcal{G}_2(g, h)) &= \frac{6149}{358}gh + \frac{587}{963}g - \frac{587}{963}h, \\
GA_5(\mathcal{G}_2(g, h)) &= \frac{7405}{206}gh - \frac{217}{1888}g - \frac{217}{1888}h.
\end{aligned} \tag{14}$$

Proof. To discover the values of these indices, the edge set must be divided into partitions depending on the sum of degrees of neighbors of end vertices of each edge. In Table 2, the partition can be observed.

The calculation of the ABC_4 index can be done in the following way:

$$\begin{aligned}
ABC_4(\mathcal{G}_2(g, h)) &= (4g + 4h)\left(\frac{423}{715}\right) + (4g + 4h)\left(\frac{462}{881}\right) \\
&\quad + (24gh - 8g - 8h)\left(\frac{702}{1457}\right) + (12gh)\left(\frac{896}{1858}\right), \\
&= \frac{6149}{358}gh + \frac{587}{963}g + \frac{587}{963}h.
\end{aligned} \tag{15}$$

TABLE 2: The degree sum of the neighbor vertices of each edge's end vertices is used to partition the graph $\mathcal{G}_2(g, h)$.

(S_s, S_t) where $st \in E(\mathcal{G}_2(g, h))$	Number of edges
(4, 5)	$4g + 4h$
(5, 8)	$4g + 4h$
(7, 8)	$24gh - 8g - 8h$
(8, 8)	$12gh$

Similarly, the fifth type of geometric-arithmetic index GA_5 can be calculated as follows:

$$\begin{aligned}
GA_5(\mathcal{G}_2(g, h)) &= (4g + 4h)\left(\frac{321}{323}\right) + (4g + 4h)\left(\frac{757}{778}\right) \\
&\quad + (2a + 2b)\left(\frac{141}{143}\right) \\
&\quad + (24gh - 8g - 8h)\left(\frac{897}{899}\right) + (12gh)(1), \\
&= \frac{7405}{206}gh - \frac{217}{1888}g - \frac{217}{1888}h.
\end{aligned} \tag{16}$$

4. Graphical Analysis and Conclusion

In this article, we have proposed some novel topological indices based on the neighborhood degree sum of end vertices of edges. Now, the results of topological indices will be compared. The comparison between the sum-connectivity index (SCI), first Zagreb index, second Zagreb index, Randic index, and hyper-Zagreb (HM) index is shown in Table 3. The graphical representation of Table 3 is given in Figure 2.

Now, the results of the metal-organic framework's atom-bond connectivity (ABC) index and geometric-arithmetic (GA) index of $TM_3C_{12}S_{12}$ will be compared as shown in Table 4. The graphical explanation of Table 4 is given in Figure 3.

Similarly, the results of the fourth type of the atom-bond connectivity (ABC) index ABC_4 and fifth type of the GA index GA_5 are compared numerically as well as graphically. The comparison of ABC_4 and GA_5 of $TM_3C_{12}S_{12}$ is shown in Table 5. The graphical view of ABC_4 and GA_5 is shown in Figure 4.

In this paper, we have computed some physical properties of the metal-organic network in terms of topological indices; for these different TIs such as Randic, atom-bond connectivity, geometric-arithmetic, first, second, and hyper-Zagreb indices, general and sum-connectivity indices, atom-bond connectivity index, and geometric-arithmetic index are calculated. This computational work will motivate the researchers to have a clear idea about the chosen structure. The computational method considered here is useful to analyze the physicochemical properties of the stated network, cost effective, and time efficient.

TABLE 3: Comparison between SCI, Randic, M_1 , M_2 , and HM of $TM_3C_{12}S_{12}$.

(s, t)	SCI	Randic	M_1	M_2	HM
(1, 1)	159/10	229/16	188	244	1004
(2, 2)	497/8	604/11	784	1040	4336
(3, 3)	3051/22	2314/19	1788	2388	9996
(4, 4)	1719/7	4514/21	3200	4288	17984
(5, 5)	5359/14	1672/5	5020	6740	28300
(6, 6)	28617/52	3841/8	7248	9744	40944
(7, 7)	3741/5	4565/7	9884	13300	55916
(8, 8)	4882/5	13607/16	12928	17408	73216
(9, 9)	18524/15	69876/65	16380	22068	92844
(10, 10)	36571/24	10607/8	20240	27280	114800

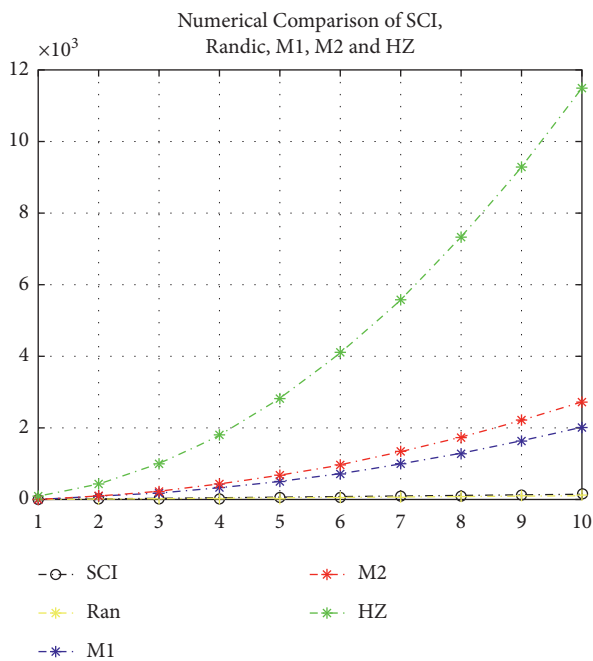


FIGURE 2: Comparison between SCI, Randic, M_1 , M_2 , and HM of $TM_3C_{12}S_{12}$.

TABLE 4: Comparison between ABC and GA of $TM_3C_{12}S_{12}$.

(s, t)	ABC	GA
(1, 1)	849/34	604/17
(2, 2)	799/8	706/5
(3, 3)	3371/15	22825/72
(4, 4)	6792/17	19141/34
(5, 5)	11861/19	12307/14
(6, 6)	15282/17	20245/16
(7, 7)	11012/9	22382/13
(8, 8)	14383/9	20234/9
(9, 9)	16181/8	25604/9
(10, 10)	44947/18	35117/10

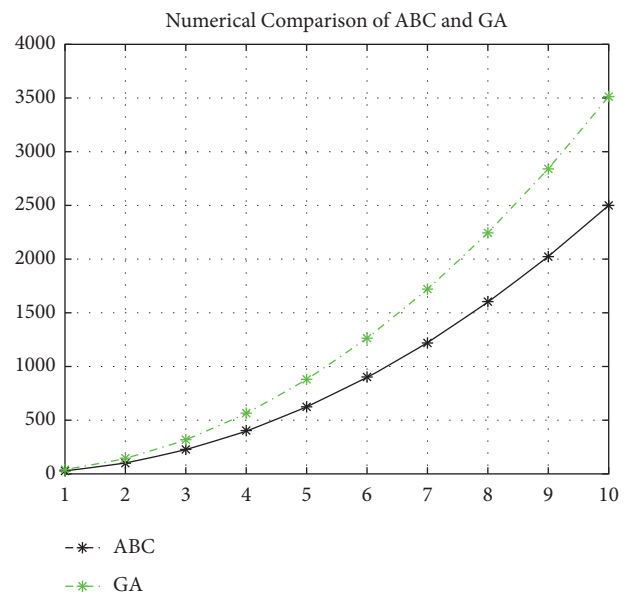


FIGURE 3: Comparison between ABC and GA of $TM_3C_{12}S_{12}$.

TABLE 5: Comparison between ABC_4 and GA_5 of $TM_3C_{12}S_{12}$.

(s, t)	ABC_4	GA_5
(1, 1)	92/5	250/7
(2, 2)	498/7	430/3
(3, 3)	4589/29	1937/6
(4, 4)	3636/13	5168/9
(5, 5)	871/2	27823/31
(6, 6)	12513/20	12927/10
(7, 7)	16153/19	15838/9
(8, 8)	72086/65	9195/4
(9, 9)	12620/9	14548/5
(10, 10)	32866/19	39516/11

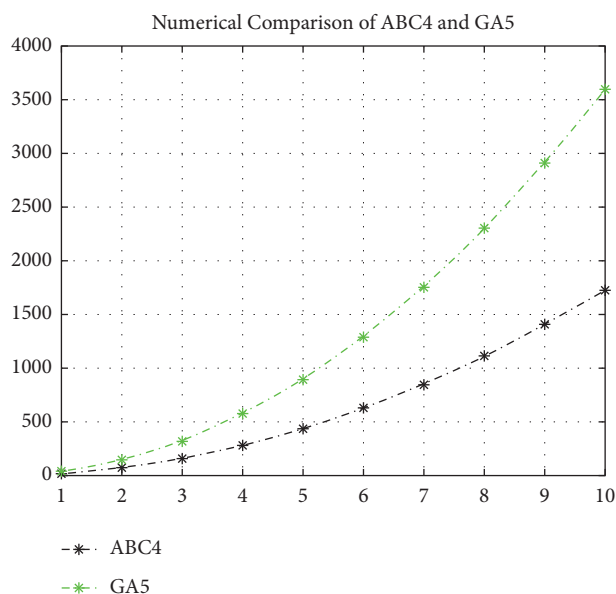


FIGURE 4: Comparison between ABC_4 and GA_5 of $TM_3C_{12}S_{12}$.

Data Availability

No data were used in this manuscript.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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