Research Article

On Ve-Degree-Based Irregularity Properties of the Crystallographic Structure of Molecules

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Irregularity indices are usually used for quantitative characterization of the topological structure of nonregular graphs. In numerous applications and problems in material engineering and chemistry, it is useful to be aware that how irregular a molecular structure is? In this paper, we are interested in formulating closed forms of irregularity measures of some of the crystallographic structures of $\text{Cu}_2\text{O}[p, q, r]$ and crystallographic structure of titanium difluoride of $T_iF_2[p, q, r]$. These theoretical conclusions provide practical guiding significance for pharmaceutical engineering and complex network and quantify the degree of folding of long organic molecules.

1. Introduction

In the medicines mathematical model, the structure of medication is taken as an undirected graph, where vertices and edges are taken as atoms and chemical bonds. Mathematical chemistry gives tools, for example, polynomials and numbers, to obtain properties of chemical compounds without utilizing quantum mechanics [1–3]. A topological index is a numerical parameter of a graph and describes its topology. It depicts the molecular structure numerically and is utilized in the advancement of qualitative structure-activity relationships (QSARs). There are three kinds of topological indices:

- (1) Degree-based.
- (2) Distance-based.
- (3) Spectral-based.

In theoretical chemistry and biology, topological indices have been used for working out the information on molecules in the form of numerical coding. This relates to characterizing physicochemical, biological, toxicologic, pharmacologic, and other properties of chemical compounds. Thousands of molecular structure descriptors have

been suggested in order to characterize the physical and chemical properties of molecules [4–6].

Degree-based indices can be further classified in the class of irregularity indices that measure the irregularity of the given graph. Recently, Réti et al. [7, 8] showed that the graph irregularity indices are efficient in quantitative structure-property relationship (QSPR) studies of molecular graphs [9].

Let $\text{Cu}_2\text{O}[p, q, r]$ be the chemical graph of Cu_2O with $p \times q$ unit cells in the plane and r layers. Copper(I) oxide or cuprous oxide is the inorganic compound with the formula Cu_2O . Figure 1 describes the graph of the molecule Cu_2O [10]. Note that copper atoms are shown in Figure 1 by red dots and oxygen atoms are shown by blue dots. In the Cu_2O lattice graph, each copper atom is attached to two oxygen atoms, and every oxygen atom is attached to four copper atoms.

It is one of the principal oxides of copper, the other being CuO or cupric oxide. Nowadays, the crystallographic structure of the molecule Cu_2O has attracted attention due to its interesting properties, low-cost, abundance, nontoxic nature [11]. This is the main reason to choose Cu_2O and compute irregularity indices for it. Figures 1–5 represent molecular graphs of these two systems.

FIGURE 3: The graph of $\text{Cu}_2\text{O}[3, 2, 3]$. FIGURE 4: The graph of $\text{TiF}_2[1, 1, 1]$.

$$\text{IRR}_t = \text{IRR}_t(G) = \frac{1}{2} \sum_{uv \in E(G)} |d(u) - d(v)|. \quad (2)$$

$$\text{IRF} = \text{IRF}(G) = \sum_{uv \in E(G)} (d(u) - d(v))^2. \quad (3)$$

Gutman et al. [25] introduced the $\text{IRF}(G)$ irregularity index of the graph G as follows:

Simplified ways of expressing the irregularities are irregularity indices. These irregularity indices have been

FIGURE 5: The graph of $T_i F_2[4, 1, 2]$.

studied recently in a novel way [26, 27]. The first such irregularity index was introduced in [28]. Table 1 shows the rest of the irregularity indices used in this paper.

Most of the well-known degree-based irregularity indices can be obtained from the following general setting:

$$\text{IR}(G) = \sum_{uv \in E(G)} f(d(u), d(v)), \quad (4)$$

where $f(d(u), d(v))$ is an appropriately selected function.

2. Results for the Crystallographic Structure

In this section, we will compute the irregularity indices of some popular crystallographic structure of molecules $\text{Cu}_2\text{O}[p, q, r]$.

From [18], we know that the graph $\text{Cu}_2\text{O}[p, q, r]$ contains $6pqr + pq + qr + pr + q + p + r + 1$ vertices and $8pqr$ edges.

We begin with obtaining formulas for irregularity measures of $\text{IRR}(\text{Cu}_2\text{O}[p, q, r])$, $\text{IRR}_t(\text{Cu}_2\text{O}[p, q, r])$, and $\text{IRF}(\text{Cu}_2\text{O}[p, q, r])$.

Theorem 1. Let $\text{Cu}_2\text{O}[p, q, r]$ be the crystallographic structure. Then, the irregularity indices of $\text{Cu}_2\text{O}[p, q, r]$ are

$$\begin{aligned} \text{IRR}(\text{Cu}_2\text{O}[p, q, r]) &= 16pqr - 8qr - 8pq - 8pr + 12p \\ &\quad + 12q + 12r - 16, \end{aligned} \quad (5)$$

$$\begin{aligned} \text{IRR}_t(\text{Cu}_2\text{O}[p, q, r]) &= 8pqr - 4qr - 4pq - 4pr + 6p \\ &\quad + 6q + 6r - 8, \end{aligned} \quad (6)$$

$$\begin{aligned} \text{IRF}(\text{Cu}_2\text{O}[p, q, r]) &= 32pqr - 16qr - 16pq - 16pr \\ &\quad + 20p + 20q + 20r - 24. \end{aligned} \quad (7)$$

Proof. Consider the graph crystallographic structure $\text{Cu}_2\text{O}[p, q, r]$. From the graph of $\text{Cu}_2\text{O}[p, q, r]$ crystallographic structure, we can see that there are three partitions, $V_{\{1\}} = \{v \in V(\text{Cu}_2\text{O}[p, q, r]) | d_v = 1\}$, $V_{\{2\}} = \{v \in V(\text{Cu}_2\text{O}[p, q, r]) | d_v = 2\}$, and $V_{\{3\}} = \{v \in V(\text{Cu}_2\text{O}[p, q, r]) | d_v = 4\}$. The edge set of $\text{Cu}_2\text{O}[p, q, r]$ can be partitioned as follows:

$$\begin{aligned} E_1 &= \{e = uv \in E(\text{Cu}_2\text{O}[p, q, r]) | d(u) = 1 \text{ and } d(v) = 2\}, \\ E_2 &= \{e = uv \in E(\text{Cu}_2\text{O}[p, q, r]) | d(u) = 2 \text{ and } d(v) = 2\}, \\ E_3 &= \{e = uv \in E(\text{Cu}_2\text{O}[p, q, r]) | d(u) = 2 \text{ and } d(v) = 4\}. \end{aligned} \quad (8)$$

From the molecular graph of $\text{Cu}_2\text{O}[p, q, r]$, we can observe in Figures 1–5 that $|E_1| = 4p + 4q + 4r - 8$, $|E_2| = 4pq + 4pr + 4qr - 8p - 8q - 8r + 12$, and $|E_3| = 4(2pqr - pq - pr - qr + p + q + r - 1)$. Thus, by the definition of Albertson index for $\text{Cu}_2\text{O}[p, q, r]$, we have

$$\begin{aligned} \text{IRR}(\text{Cu}_2\text{O}[p, q, r]) &= \sum_{uv \in E(\text{Cu}_2\text{O}[p, q, r])} |d(u) - d(v)| \\ &= \sum_{uv \in E_1(\text{Cu}_2\text{O}[p, q, r])} d(u) - d(v) + \sum_{uv \in E_2(\text{Cu}_2\text{O}[p, q, r])} |d(u) - d(v)| + \sum_{uv \in E_3(\text{Cu}_2\text{O}[p, q, r])} d(u) - d(v) \\ &= (4p + 4q + 4r - 8) \times |1 - 2| + 4(2pqr - pq - pr - qr + p + q + r - 1) \times |2 - 4| \\ &= 16pqr - 8qr - 8pq - 8pr + 12p + 12q + 12r - 16, \end{aligned} \quad (9)$$

TABLE 1: Some irregularity indices considered in [8].

Symbol	Irregularity indices	The function $f(d(u), d(v))$ in equation (28)
IRDIF		$(d(u)/d(v) - d(v)/d(u))$
IRL		$(\ln d(u) - \ln d(v))$
IRLU		$ d(u) - d(v) /\min(d(u), d(v))$
IRLF		$ d(u) - d(v) /\sqrt{(d(u) \times d(v))}$
IRLA		$2 d(u) - d(v) /d(u) + d(v)$
$IRLD_1$		$\ln\{1 + d(u) - d(v) \}$
IRGA		$\ln(d(u) - d(v) /\sqrt{(d(u) \times d(v))})$
IRA		$(d(u)^{-1/2} - d(v)^{-1/2})^2$
IRB		$(d(u)^{1/2} - d(v)^{1/2})^2$

which is the required formula result (5).

By the definition of total irregularity measure of $\text{Cu}_2\text{O}[p, q, r]$, we have

$$\begin{aligned}
 \text{IRR}_t(\text{Cu}_2\text{O}[p, q, r]) &= \frac{1}{2} \sum_{uv \in E(\text{Cu}_2\text{O}[p, q, r])} |d(u) - d(v)| \\
 &= \frac{1}{2} \sum_{uv \in E_1(\text{Cu}_2\text{O}[p, q, r])} |d(u) - d(v)| + \frac{1}{2} \sum_{uv \in E_2(\text{Cu}_2\text{O}[p, q, r])} |d(u) - d(v)| + \frac{1}{2} \sum_{uv \in E_3(\text{Cu}_2\text{O}[p, q, r])} |d(u) - d(v)| \\
 &= \frac{1}{2} \times (4p + 4q + 4r - 8) \times |1 - 2| + \frac{1}{2} \times 4(2pqr - pq - pr - qr + p + q + r - 1) \times |2 - 4| \\
 &= 8pqr - 4qr - 4pq - 4pr + 6p + 6q + 6r - 8,
 \end{aligned} \tag{10}$$

which is the required formula result (7).

By the definition of irregularity index IRF for $\text{Cu}_2\text{O}[p, q, r]$, we have

$$\begin{aligned}
 \text{IRF}(\text{Cu}_2\text{O}[p, q, r]) &= \sum_{uv \in E(\text{Cu}_2\text{O}[p, q, r])} (d(u) - d(v))^2 \\
 &= \sum_{uv \in E_1(\text{Cu}_2\text{O}[p, q, r])} (d(u) - d(v))^2 + \sum_{uv \in E_2(\text{Cu}_2\text{O}[p, q, r])} (d(u) - d(v))^2 + \sum_{uv \in E_3(\text{Cu}_2\text{O}[p, q, r])} (d(u) - d(v))^2 \\
 &= (4p + 4q + 4r - 8) \times (1 - 2)^2 + 4(2pqr - pq - pr - qr + p + q + r - 1) \times (2 - 4)^2 \\
 &= 32pqr - 16qr - 16pq - 16pr + 20p + 20q + 20r - 24,
 \end{aligned} \tag{11}$$

which is the required formula result (8).

Note that throughout the paper, colors red, blue, and green represent IRR, IRR_t , and IRF, respectively.

The next example represents some values of the calculated irregularity indices of $\text{IRR}(\text{Cu}_2\text{O}[p, q, r])$, $\text{IRR}_t(\text{Cu}_2\text{O}[p, q, r])$, and $\text{IRF}(\text{Cu}_2\text{O}[p, q, r])$ for some test values of $p = q = r = 1$. $\square$

Example 1. Let $\text{Cu}_2\text{O}[1, 1, 1]$ be crystallographic structure described in Figure 2. Then,

$$\begin{aligned}
 \text{IRR}(\text{Cu}_2\text{O}[1, 1, 1]) &= 12, \\
 \text{IRR}_t(\text{Cu}_2\text{O}[1, 1, 1]) &= 6, \\
 \text{IRF}(\text{Cu}_2\text{O}[1, 1, 1]) &= 20.
 \end{aligned} \tag{12}$$

Theorem 2. Let $\text{Cu}_2\text{O}[p, q, r]$ be the crystallographic structure. Then, the irregularity indices of $\text{Cu}_2\text{O}[p, q, r]$ are

$$\begin{aligned} \text{IRL}(\text{Cu}_2\text{O}[p, q, r]) &= 5.5451774444792pqr - 2.7725887222396qr - 2.7725887222396pq - 2.7725887222396pr \\ &\quad + 5.5451774444792p + 5.5451774444792q + 5.5451774444792r - 8.3177661667188. \\ \text{IRD}_1(\text{Cu}_2\text{O}[p, q, r]) &= 8.7888983093448pqr - 4.3944491546724pq - 4.3944491546724pr - 4.3944491546724qr \\ &\quad + 7.167037876912p + 7.167037876912q + 7.167037876912r - 9.9396265991516. \\ \text{IRGA}(\text{Cu}_2\text{O}[p, q, r]) &= 1.8845285705024pqr - 0.9422642852512pq - 0.9422642852512pr - 0.9422642852512qr \\ &\quad + 1.177830356564p + 1.177830356564q + 1.177830356564r - 0.7066982139384. \end{aligned} \quad (13)$$

Proof. By definition of IRL irregularity index of $\text{Cu}_2\text{O}[p, q, r]$, we have

$$\begin{aligned} \text{IRL}(\text{Cu}_2\text{O}[p, q, r]) &= \sum_{uv \in E(\text{Cu}_2\text{O}[p, q, r])} |\ln d(u) - \ln d(v)| \\ &= \sum_{uv \in E_1(\text{Cu}_2\text{O}[p, q, r])} |\ln d(u) - \ln d(v)| + \sum_{uv \in E_2(\text{Cu}_2\text{O}[p, q, r])} |\ln d(u) - \ln d(v)| \\ &\quad + \sum_{uv \in E_3(\text{Cu}_2\text{O}[p, q, r])} |\ln d(u) - \ln d(v)| \\ &= (4p + 4q + 4r - 8) \times |\ln 1 - \ln 2| + 4(2pqr - pq - pr - qr + p + q + r - 1) \\ &\quad \times |\ln 2 - \ln 4| = 5.5451774444792pqr - 2.7725887222396qr - 2.7725887222396pq - 2.7725887222396pr \\ &\quad + 5.5451774444792p + 5.5451774444792q + 5.5451774444792r - 8.3177661667188. \end{aligned} \quad (14)$$

By applying the definition of IRD_1 for $\text{Cu}_2\text{O}[p, q, r]$, we have

$$\begin{aligned} \text{IRD}_1(\text{Cu}_2\text{O}[p, q, r]) &= \sum_{uv \in E(\text{Cu}_2\text{O}[p, q, r])} \ln\{1 + |d(u) - d(v)|\} \\ &= \sum_{uv \in E_1(\text{Cu}_2\text{O}[p, q, r])} \ln\{1 + |d(u) - d(v)|\} \\ &\quad + \sum_{uv \in E_2(\text{Cu}_2\text{O}[p, q, r])} \ln\{1 + |d(u) - d(v)|\} \\ &\quad + \sum_{uv \in E_3(\text{Cu}_2\text{O}[p, q, r])} \ln\{1 + |d(u) - d(v)|\} \\ &= (4p + 4q + 4r - 8) \times \ln\{1 + |1 - 2|\} + 4(2pqr - pq - pr - qr + p + q + r - 1) \times \ln\{1 + |2 - 4|\} \\ &= 8.7888983093448pqr - 4.3944491546724pq - 4.3944491546724pr - 4.3944491546724qr \\ &\quad + 7.167037876912p + 7.167037876912q + 7.167037876912r - 9.9396265991516. \end{aligned} \quad (15)$$

Finally, by applying the definition of IRGA for $\text{Cu}_2\text{O}[p, q, r]$, we have

$$\begin{aligned}
\text{IRGA}(\text{Cu}_2\text{O}[p, q, r]) &= \sum_{uv \in E(\text{Cu}_2\text{O}[p, q, r])} \ln\left(\frac{d(u) + d(v)}{2\sqrt{d(u) \times d(v)}}\right) \\
&= \sum_{uv \in E_1(\text{Cu}_2\text{O}[p, q, r])} \ln\left(\frac{d(u) + d(v)}{2\sqrt{d(u) \times d(v)}}\right) + \sum_{uv \in E_2(\text{Cu}_2\text{O}[p, q, r])} \ln\left(\frac{d(u) + d(v)}{2\sqrt{d(u) \times d(v)}}\right) \\
&\quad + \sum_{uv \in E_3(\text{Cu}_2\text{O}[p, q, r])} \ln\left(\frac{d(u) + d(v)}{2\sqrt{d(u) \times d(v)}}\right) \\
&= (4p + 4q + 4r - 8) \times \ln\frac{1+2}{2\sqrt{1 \times 2}} + (4pq + 4pr + 4qr - 8p - 8q - 8r + 12) \times \ln\frac{2+2}{2\sqrt{2 \times 2}} \\
&\quad + 4(2pqr - pq - pr - qr + p + q + r - 1) \times \ln\frac{2+4}{2\sqrt{2 \times 4}} \\
&= 1.8845285705024pqr - 0.9422642852512pq - 0.9422642852512pr \\
&\quad - 0.9422642852512qr + 1.177830356564p + 1.177830356564q + 1.177830356564r \\
&\quad - 0.7066982139384.
\end{aligned} \tag{16}$$

Note that throughout the paper, colors violet, yellow, and Peru represent IRL, IRD_1 , and IRGA, respectively. $\square$

Theorem 3. Let $\text{Cu}_2\text{O}[p, q, r]$ be the crystallographic structure. Then, the irregularity indices of $\text{Cu}_2\text{O}[p, q, r]$ are

$$\begin{aligned}
\text{IRA}(\text{Cu}_2\text{O}[p, q, r]) &= (4p + 4q + 4r - 8) \times \left(\frac{3}{2} - \sqrt{2}\right) + (2pqr - pq - pr - qr + p + q + r - 1) \times (3 - 2\sqrt{2}), \\
\text{IRB}(\text{Cu}_2\text{O}[p, q, r]) &= (4p + 4q + 4r - 8) \times (3 - 2\sqrt{2}) + (2pqr - pq - pr - qr + p + q + r - 1) \times (24 - 16\sqrt{2}), \\
\text{IRDIF}(\text{Cu}_2\text{O}[p, q, r]) &= 12pqr - 6qr - 6pq - 6pr + 12p + 12q + 12r - 18.
\end{aligned} \tag{17}$$

Proof. By applying the definition of IRA for $\text{Cu}_2\text{O}[p, q, r]$, we have

$$\begin{aligned}
\text{IRA}(\text{Cu}_2\text{O}[p, q, r]) &= \sum_{uv \in E(\text{Cu}_2\text{O}[p, q, r])} \left(\sqrt{\frac{1}{d(u)}} - \sqrt{\frac{1}{d(v)}} \right)^2 \\
&= \sum_{uv \in E_1(\text{Cu}_2\text{O}[p, q, r])} \left(\sqrt{\frac{1}{d(u)}} - \sqrt{\frac{1}{d(v)}} \right)^2 + \sum_{uv \in E_2(\text{Cu}_2\text{O}[p, q, r])} \left(\sqrt{\frac{1}{d(u)}} - \sqrt{\frac{1}{d(v)}} \right)^2 \\
&\quad + \sum_{uv \in E_3(\text{Cu}_2\text{O}[p, q, r])} \left(\sqrt{\frac{1}{d(u)}} - \sqrt{\frac{1}{d(v)}} \right)^2 \\
&= (4p + 4q + 4r - 8) \times \left(\sqrt{1} - \sqrt{\frac{1}{2}} \right)^2 + 4(2pqr - pq - pr - qr + p + q + r - 1) \times \left(\sqrt{\frac{1}{2}} - \sqrt{\frac{1}{4}} \right)^2 \\
&= (4p + 4q + 4r - 8) \times \left(\frac{3}{2} - \sqrt{2} \right) + (2pqr - pq - pr - qr + p + q + r - 1) \times (3 - 2\sqrt{2}).
\end{aligned} \tag{18}$$

By applying the definition of IRB for $\text{Cu}_2\text{O}[p, q, r]$, we have

$$\begin{aligned}
 \text{IRB}(\text{Cu}_2\text{O}[p, q, r]) &= \sum_{uv \in E(\text{Cu}_2\text{O}[p, q, r])} (\sqrt{d(u)} - \sqrt{d(v)})^2 \\
 &= \sum_{uv \in E_1(\text{Cu}_2\text{O}[p, q, r])} (\sqrt{d(u)} - \sqrt{d(v)})^2 \\
 &\quad + \sum_{uv \in E_2(\text{Cu}_2\text{O}[p, q, r])} (\sqrt{d(u)} - \sqrt{d(v)})^2 + \sum_{uv \in E_3(\text{Cu}_2\text{O}[p, q, r])} (\sqrt{d(u)} - \sqrt{d(v)})^2 \\
 &= (4p + 4q + 4r - 8) \times (\sqrt{1} - \sqrt{2})^2 + 4(2pqr - pq - pr - qr + p + q + r - 1) \times (\sqrt{2} - \sqrt{4})^2 \\
 &= (4p + 4q + 4r - 8) \times (3 - 2\sqrt{2}) + (2pqr - pq - pr - qr + p + q + r - 1) \times (24 - 16\sqrt{2}).
 \end{aligned} \tag{19}$$

Finally, by applying the definition of IRDIF for $\text{Cu}_2\text{O}[p, q, r]$, we have

$$\begin{aligned}
 \text{IRDIF}(\text{Cu}_2\text{O}[p, q, r]) &= \sum_{uv \in E(\text{Cu}_2\text{O}[p, q, r])} \left| \frac{d(u)}{d(v)} - \frac{d(v)}{d(u)} \right| \\
 &= \sum_{uv \in E_1(\text{Cu}_2\text{O}[p, q, r])} \left| \frac{d(u)}{d(v)} - \frac{d(v)}{d(u)} \right| + \sum_{uv \in E_2(\text{Cu}_2\text{O}[p, q, r])} \left| \frac{d(u)}{d(v)} - \frac{d(v)}{d(u)} \right| + \sum_{uv \in E_3(\text{Cu}_2\text{O}[p, q, r])} \left| \frac{d(u)}{d(v)} - \frac{d(v)}{d(u)} \right| \\
 &= (4p + 4q + 4r - 8) \times \left| \frac{1}{2} - \frac{2}{1} \right| + 4(2pqr - pq - pr - qr + p + q + r - 1) \times \left| \frac{2}{4} - \frac{4}{2} \right| \\
 &= 12pqr - 6qr - 6pq - 6pr + 12p + 12q + 12r - 18.
 \end{aligned} \tag{20}$$

Note that throughout the paper, colors aquamarine, black, and blue violet represent IRA, IRB, and IRDIF, respectively. $\square$

Theorem 4. Let $\text{Cu}_2\text{O}[p, q, r]$ be the crystallographic structure. Then, the irregularity indices of $\text{Cu}_2\text{O}[p, q, r]$ are

$$\begin{aligned}
 \text{IRLU}(\text{Cu}_2\text{O}[p, q, r]) &= 8pqr - 4qr - 4pq - 4pr + 8p + 8q + 8r - 12, \\
 \text{IRLA}(\text{Cu}_2\text{O}[p, q, r]) &= \frac{8pqr}{3} - \frac{4qr}{3} - \frac{4pq}{3} - \frac{4pr}{3} + \frac{8p}{3} + \frac{8q}{3} + \frac{8r}{3} - 4, \\
 \text{IRLF}(\text{Cu}_2\text{O}[p, q, r]) &= (4p + 4q + 4r - 8) \times \sqrt{2} + (2pqr - pq - pr - qr + p + q + r - 1) \times 2\sqrt{2}.
 \end{aligned} \tag{21}$$

Proof. By definition of IRLU irregularity index of $\text{Cu}_2\text{O}[p, q, r]$, we have

$$\begin{aligned}
\text{IRLU}(\text{Cu}_2\text{O}[p, q, r]) &= \sum_{uv \in E(\text{Cu}_2\text{O}[p, q, r])} \frac{|d(u) - d(v)|}{\min(d(u), d(v))} \\
&= \sum_{uv \in E_1(\text{Cu}_2\text{O}[p, q, r])} \frac{|d(u) - d(v)|}{\min(d(u), d(v))} + \sum_{uv \in E_2(\text{Cu}_2\text{O}[p, q, r])} \frac{|d(u) - d(v)|}{\min(d(u), d(v))} \\
&\quad + \sum_{uv \in E_3(\text{Cu}_2\text{O}[p, q, r])} \frac{|d(u) - d(v)|}{\min(d(u), d(v))} \\
&= (4p + 4q + 4r - 8) \times \frac{|1 - 2|}{\min(1, 2)} + 4(2pqr - pq - pr - qr + p + q + r - 1) \times \frac{|2 - 4|}{\min(2, 4)} \\
&= 8pqr - 4qr - 4pq - 4pr + 8p + 8q + 8r - 12.
\end{aligned} \tag{22}$$

By applying the definition of IRLA for $\text{Cu}_2\text{O}[p, q, r]$, we have

$$\begin{aligned}
\text{IRLA}(\text{Cu}_2\text{O}[p, q, r]) &= \sum_{uv \in E(\text{Cu}_2\text{O}[p, q, r])} 2 \frac{|d(u) - d(v)|}{(d(u) + d(v))} \\
&= \sum_{uv \in E_1(\text{Cu}_2\text{O}[p, q, r])} 2 \frac{|d(u) - d(v)|}{(d(u) + d(v))} + \sum_{uv \in E_2(\text{Cu}_2\text{O}[p, q, r])} 2 \frac{|d(u) - d(v)|}{(d(u) + d(v))} + \sum_{uv \in E_3(\text{Cu}_2\text{O}[p, q, r])} 2 \frac{|d(u) - d(v)|}{(d(u) + d(v))} \\
&= (4p + 4q + 4r - 8) \times \frac{|1 - 2|}{(1 + 2)} + 4(2pqr - pq - pr - qr + p + q + r - 1) \times \frac{|2 - 4|}{(2 + 4)} = \frac{8pqr}{3} \\
&\quad - \frac{4qr}{3} - \frac{4pq}{3} - \frac{4pr}{3} + \frac{8p}{3} + \frac{8q}{3} + \frac{8r}{3} - 4.
\end{aligned} \tag{23}$$

By applying the definition of IRLF for $\text{Cu}_2\text{O}[p, q, r]$, we have

$$\begin{aligned}
\text{IRLF}(\text{Cu}_2\text{O}[p, q, r]) &= \sum_{uv \in E(\text{Cu}_2\text{O}[p, q, r])} \frac{|d(u) - d(v)|}{\sqrt{d(u) \times d(v)}} \\
&= \sum_{uv \in E_1(\text{Cu}_2\text{O}[p, q, r])} \frac{|d(u) - d(v)|}{\sqrt{d(u) \times d(v)}} + \sum_{uv \in E_2(\text{Cu}_2\text{O}[p, q, r])} \frac{|d(u) - d(v)|}{\sqrt{d(u) \times d(v)}} + \sum_{uv \in E_3(\text{Cu}_2\text{O}[p, q, r])} \frac{|d(u) - d(v)|}{\sqrt{d(u) \times d(v)}} \\
&= (4p + 4q + 4r - 8) \times \frac{|1 - 2|}{\sqrt{1 \times 2}} + 4(2pqr - pq - pr - qr + p + q + r - 1) \times \frac{|2 - 4|}{\sqrt{2 \times 4}} \\
&= (4p + 4q + 4r - 8) \times \sqrt{2} \\
&\quad + (2pqr - pq - pr - qr + p + q + r - 1) \times 2\sqrt{2}.
\end{aligned} \tag{24}$$

Note that throughout the paper, colors dark orange, fuchsia, and gray represent IRLU, IRLA, and IRLF, respectively.

Next example represents some values of the calculated irregularity indices of $\text{IRLU}(\text{Cu}_2\text{O}[p, q, r])$, $\text{IRLA}(\text{Cu}_2\text{O}[p, q, r])$, $\text{IRLF}(\text{Cu}_2\text{O}[p, q, r])$, and IRDIF

$(\text{Cu}_2\text{O}[p, q, r])$ for some test values of $p = 3, q = 2$, and $r = 3$. $\square$

Example 2. Let $\text{Cu}_2\text{O}[3, 2, 3]$ be crystallographic structure described in Figure 3.

Then,

$$\begin{aligned} \text{IRLU}(\text{Cu}_2\text{O}[3, 2, 3]) &= 112, \\ \text{IRLA}(\text{Cu}_2\text{O}[3, 2, 3]) &= 37.33333333333333, \\ \text{IRLF}(\text{Cu}_2\text{O}[3, 2, 3]) &= 79.1959594928933, \\ \text{IRDIF}(\text{Cu}_2\text{O}[3, 2, 3]) &= 168. \end{aligned} \quad (25)$$

3. Results for the Crystallographic Structure of Titanium Difluoride

In this section, we compute irregularity measures of crystal structure of titanium difluoride of $T_iF_2[p, q, r]$.

Titanium difluoride is a water-insoluble titanium hot-spot for use in oxygen-delicate applications, for example, metal generation. The concoction chart of the crystallographic structure of $T_iF_2[p, q, r]$ is depicted in Figure 1 graph unit cell of Cu_2O (see [29]). In Figures 4 and 5, red dots are for F atoms and green dots are for T_i atoms.

From [18], we know that the graph $T_iF_2[p, q, r]$ contains $12pqr + 2pq + 2pr + 2qr + p + q + r + 1$ vertices and $32pqr$ edges.

Here, we obtain some formulas for irregularity measures of $\text{IRR}(T_iF_2[p, q, r])$, $\text{IRR}_t(T_iF_2[p, q, r])$, and $\text{IRF}(T_iF_2[p, q, r])$.

Theorem 5. Let $T_iF_2[p, q, r]$ be the crystallographic structure of titanium difluoride. Then, the irregularity indices of $T_iF_2[p, q, r]$ are

$$\text{IRR}(T_iF_2[p, q, r]) = 128pqr - 64qr - 64pq - 64pr + 48p + 48q + 48r - 56, \quad (26)$$

$$\text{IRR}_t(T_iF_2[p, q, r]) = 64pqr - 32qr - 32pq - 32pr + 24p + 24q + 24r - 28, \quad (27)$$

$$\text{IRF}(T_iF_2[p, q, r]) = 512pqr - 256qr - 256pq - 256pr + 160p + 160q + 160r - 152. \quad (28)$$

Proof. Consider the graph crystallographic structure of titanium difluoride $T_iF_2[p, q, r]$. From the graph of $T_iF_2[p, q, r]$ crystallographic structure of titanium difluoride, we can see that there are four partitions, $V_{\{1\}} = \{v \in V(T_iF_2[p, q, r]) | d(v) = 1\}$,

$V_{\{2\}} = \{v \in V(T_iF_2[p, q, r]) | d(v) = 2\}$, $V_{\{3\}} = \{v \in V(T_iF_2[p, q, r]) | d(v) = 4\}$, and $V_{\{4\}} = \{v \in V(T_iF_2[p, q, r]) | d(v) = 8\}$. The edge set of $T_iF_2[p, q, r]$ can be partitioned as follows:

$$\begin{aligned} E_1 &= \{e = uv \in E(T_iF_2[p, q, r]) | d(u) = 1 \text{ and } d(v) = 4\}, \\ E_2 &= \{e = uv \in E(T_iF_2[p, q, r]) | d(u) = 2 \text{ and } d(v) = 4\}, \\ E_3 &= \{e = uv \in E(T_iF_2[p, q, r]) | d(u) = 4 \text{ and } d(v) = 4\}, \\ E_4 &= \{e = uv \in E(T_iF_2[p, q, r]) | d(u) = 4 \text{ and } d(v) = 8\}. \end{aligned} \quad (29)$$

From the molecular graph of $T_iF_2[p, q, r]$, we can observe in Figures 4 and 5 that $|E_1| = 8$, $|E_2| = 8(p + q + r - 3)$, $|E_3| = 16(pq + pr + qr) - 16(p + q + r) + 24$, and $|E_4| =$

$32pqr - 16(pq + pr + qr) + 8(p + q + r) - 8$. By applying the definition of Albertson index for $T_iF_2[p, q, r]$, we have

$$\begin{aligned} \text{IRR}(T_iF_2[p, q, r]) &= \sum_{uv \in E(T_iF_2[p, q, r])} |d(u) - d(v)| \\ &= \sum_{uv \in E_1(T_iF_2[p, q, r])} |d(u) - d(v)| + \sum_{uv \in E_2(T_iF_2[p, q, r])} |d(u) - d(v)| + \sum_{uv \in E_3(T_iF_2[p, q, r])} |d(u) - d(v)| \\ &\quad + \sum_{uv \in E_4(T_iF_2[p, q, r])} |d(u) - d(v)| \\ &= 8 \times |1 - 4| + 8(p + q + r - 3) \times |2 - 4| + (32pqr - 16(pq + pr + qr)) + (8(p + q + r) - 8) \times |4 - 8| \\ &= 128pqr - 64qr - 64pq - 64pr + 48p + 48q + 48r - 56, \end{aligned} \quad (30)$$

which is the required result (26). By applying the definition of total irregularity measure for $T_iF_2[p, q, r]$, we have

$$\begin{aligned}
 \text{IRR}_t(\text{Cu}_2\text{O}[p, q, r]) &= \frac{1}{2} \sum_{uv \in E(T_iF_2[p, q, r])} |d(u) - d(v)| \\
 &= \frac{1}{2} \sum_{uv \in E_1(T_iF_2[p, q, r])} |d(u) - d(v)| + \frac{1}{2} \sum_{uv \in E_2(T_iF_2[p, q, r])} |d(u) - d(v)| + \frac{1}{2} \sum_{uv \in E_3(T_iF_2[p, q, r])} |d(u) - d(v)| \\
 &\quad + \frac{1}{2} \sum_{uv \in E_4(T_iF_2[p, q, r])} |d(u) - d(v)| \\
 &= \frac{1}{2} \times 8 \times |1 - 4| + \frac{1}{2} \times 8(p + q + r - 3) \times |2 - 4| + (32pqr - 16(pq + pr + qr)) \\
 &\quad + (8(p + q + r) - 8) \times \frac{1}{2} \times |4 - 8| \\
 &= 64pqr - 32qr - 32pq - 32pr + 24p + 24q + 24r - 28,
 \end{aligned} \tag{31}$$

which is the required result (27).

By applying the definition of IRF for $T_iF_2[p, q, r]$, we have

$$\begin{aligned}
 \text{IRF}(T_iF_2[p, q, r]) &= \sum_{uv \in E(T_iF_2[p, q, r])} (d(u) - d(v))^2 \\
 &= \sum_{uv \in E_1(T_iF_2[p, q, r])} (d(u) - d(v))^2 + \sum_{uv \in E_2(CT_iF_2[p, q, r])} (d(u) - d(v))^2 + \sum_{uv \in E_3(T_iF_2[p, q, r])} (d(u) - d(v))^2 \\
 &\quad + \sum_{uv \in E_4(T_iF_2[p, q, r])} (d(u) - d(v))^2 \\
 &= 8 \times (1 - 4)^2 + 8(p + q + r - 3) \times (2 - 4)^2 + (32pqr - 16(pq + pr + qr) + (8(p + q + r) - 8) \times (4 - 8)^2 \\
 &= 512pqr - 256qr - 256pq - 256pr + 160p + 160q + 160r - 152,
 \end{aligned} \tag{32}$$

which is the required result (28).

The next example represents some values of the calculated irregularity indices of $\text{IRAL}(T_iF_2[p, q, r])$, $\text{IRR}_t(T_iF_2[p, q, r])$, and $\text{IRF}(T_iF_2[p, q, r])$ for some test values of $p = q = r = 1$. $\square$

Example 3. Let $T_iF_2[1, 1, 1]$ be the crystallographic structure of titanium difluoride described in Figure 4. Then,

$$\begin{aligned}
 \text{IRAL}(T_iF_2[1, 1, 1]) &= 24, \\
 \text{IRR}_t(T_iF_2[1, 1, 1]) &= 12, \\
 \text{IRF}(T_iF_2[1, 1, 1]) &= 72.
 \end{aligned} \tag{33}$$

Theorem 6. Let $T_iF_2[p, q, r]$ be the crystallographic structure of titanium difluoride. Then, the irregularity indices of $T_iF_2[p, q, r]$ are

$$\begin{aligned}
\text{IRL}(T_i F_2[p, q, r]) &= 22.1807097779168pqr - 11.0903548889584qr - 11.0903548889584pq - 11.0903548889584pr \\
&\quad + 11.0903548889584p + 11.0903548889584q + 11.0903548889584r - 11.0903548889576, \\
\text{IRD}_1(T_i F_2[p, q, r]) &= 51.5020131978912pqr - 25.7510065989456pq - 25.7510065989456pr - 25.7510065989456qr \\
&\quad + 21.6644016088176p + 21.6644016088176q + 21.6644016088176r - 28.151843338548, \\
\text{IRGA}(T_i F_2[p, q, r]) &= 1.8845285705024pqr - 0.9422642852512pq - 0.9422642852512pr - 0.9422642852512qr \\
&\quad + 1.177830356564p + 1.177830356564q + 1.177830356564r - 0.0993801599888.
\end{aligned} \tag{34}$$

Proof. By applying the definition of IRL for $T_i F_2[p, q, r]$, we have

$$\begin{aligned}
\text{IRL}(T_i F_2[p, q, r]) &= \sum_{uv \in E(T_i F_2[p, q, r])} |\ln d(u) - \ln d(v)| \\
&= \sum_{uv \in E_1(T_i F_2[p, q, r])} |\ln d(u) - \ln d(v)| + \sum_{uv \in E_2(T_i F_2[p, q, r])} |\ln d(u) - \ln d(v)| \\
&\quad + \sum_{uv \in E_3(T_i F_2[p, q, r])} |\ln d(u) - \ln d(v)| \\
&= 8 \times |\ln 1 - \ln 4| + 8(p + q + r - 3) \times |\ln 2 - \ln 4| + (32pqr - 16(pq + pr + qr) \\
&\quad + (8(p + q + r) - 8) \times |\ln 4 - \ln 8| \\
&= 22.1807097779168pqr - 11.0903548889584qr - 11.0903548889584pq - 11.0903548889584pr \\
&\quad + 11.0903548889584p + 11.0903548889584q + 11.0903548889584r - 11.0903548889576.
\end{aligned} \tag{35}$$

By applying the definition of IRD_1 for $T_i F_2[p, q, r]$, we have

$$\begin{aligned}
\text{IRD}_1(T_i F_2[p, q, r]) &= \sum_{uv \in E(T_i F_2[p, q, r])} \ln\{1 + |d(u) - d(v)|\} \\
&= \sum_{uv \in E_1(T_i F_2[p, q, r])} \ln\{1 + |d(u) - d(v)|\} + \sum_{uv \in E_2(T_i F_2[p, q, r])} \ln\{1 + |d(u) - d(v)|\} \\
&\quad + \sum_{uv \in E_3(T_i F_2[p, q, r])} \ln\{1 + |d(u) - d(v)|\} \\
&= 8 \times \ln\{1 + |1 - 4|\} + 8(p + q + r - 3) \times \ln\{1 + |2 - 4|\} \\
&\quad + (32pqr - 16(pq + pr + qr)) + (8(p + q + r) - 8) \times \ln\{1 + |4 - 8|\} \\
&= 51.5020131978912pqr - 25.7510065989456pq - 25.7510065989456pr \\
&\quad - 25.7510065989456qr + 21.6644016088176p + 21.6644016088176q \\
&\quad + 21.6644016088176r - 28.151843338548.
\end{aligned} \tag{36}$$

Finally, by applying the definition of IRGA for $T_iF_2[p, q, r]$, we have

$$\begin{aligned}
 \text{IRGA}(T_iF_2[p, q, r]) &= \sum_{uv \in E(T_iF_2[p, q, r])} \ln \frac{d(u) + d(v)}{2\sqrt{d(u) \times d(v)}} \\
 &= \sum_{uv \in E_1(T_iF_2[p, q, r])} \ln \frac{d(u) + d(v)}{2\sqrt{d(u) \times d(v)}} + \sum_{uv \in E_2(T_iF_2[p, q, r])} \ln \frac{d(u) + d(v)}{2\sqrt{d(u) \times d(v)}} \\
 &\quad + \sum_{uv \in E_3(T_iF_2[p, q, r])} \ln \frac{d(u) + d(v)}{2\sqrt{d(u) \times d(v)}} + \sum_{uv \in E_4(T_iF_2[p, q, r])} \ln \frac{d(u) + d(v)}{2\sqrt{d(u) \times d(v)}} \\
 &= 8 \times \ln \frac{1+4}{2\sqrt{1 \times 4}} + 8(p+q+r-3) \times \ln \frac{2+4}{2\sqrt{2 \times 4}} + (16pq + 16pr + 16qr - 16p - 16q - 16r + 24) \times \\
 &\quad \times \ln \frac{4+4}{2\sqrt{4 \times 4}} + (32pqr - 16(pq + pr + qr) + (8(p+q+r-8) \times) \\
 &\quad \ln \frac{4+8}{2\sqrt{4 \times 8}} = 1.8845285705024pqr - 0.9422642852512pq - 0.9422642852512pr - 0.9422642852512qr + 1.177830356564p \\
 &\quad + 1.177830356564q + 1.177830356564r - 0.0993801599888.
 \end{aligned} \tag{37}$$

Theorem 7. Let $T_iF_2[p, q, r]$ be the crystallographic structure of titanium difluoride. Then, the irregularity indices of $T_iF_2[p, q, r]$ are

$$\begin{aligned}
 \text{IRA}(T_iF_2[p, q, r]) &= (4p + 4q + 4r - 8) \times (6 - 4\sqrt{2}) + (2pqr - pq - pr - qr + p + q + r - 1) \times \left(-\frac{\sqrt{2}}{4} + \frac{3}{8}\right) + 2, \\
 \text{IRB}(T_iF_2[p, q, r]) &= (4p + 4q + 4r - 8) \times (48 - 32\sqrt{2}) + (2pqr - pq - pr - qr + p + q + r - 1) \times (12 - 8\sqrt{2}) + 8, \\
 \text{IRDIF}(T_iF_2[p, q, r]) &= 48pqr - 24qr - 24pq - 24pr + 24p + 24q + 24r - 18.
 \end{aligned} \tag{38}$$

Proof. By applying the definition of IRA for $T_iF_2[p, q, r]$, we have

$$\begin{aligned}
\text{IRA}(T_i F_2[p, q, r]) &= \sum_{uv \in E(T_i F_2[p, q, r])} \left(\sqrt{\frac{1}{d(u)}} - \sqrt{\frac{1}{d(v)}} \right)^2 \\
&= \sum_{uv \in E_1(T_i F_2[p, q, r])} \left(\sqrt{\frac{1}{d(u)}} - \sqrt{\frac{1}{d(v)}} \right)^2 + \sum_{uv \in E_2(T_i F_2[p, q, r])} \left(\sqrt{\frac{1}{d(u)}} - \sqrt{\frac{1}{d(v)}} \right)^2 \\
&\quad + \sum_{uv \in E_3(T_i F_2[p, q, r])} \left(\sqrt{\frac{1}{d(u)}} - \sqrt{\frac{1}{d(v)}} \right)^2 + \sum_{uv \in E_4(T_i F_2[p, q, r])} \left(\sqrt{\frac{1}{d(u)}} - \sqrt{\frac{1}{d(v)}} \right)^2 \\
&= 8 \times \left(\sqrt{1} - \sqrt{\frac{1}{4}} \right)^2 + 8(p+q+r-3) \times \left(\sqrt{\frac{1}{2}} - \sqrt{\frac{1}{4}} \right)^2 + (32pqr - 16(pq + pr + (p+qqr)) + (8+r-8)) \\
&\quad \times \left(\sqrt{\frac{1}{4}} - \sqrt{\frac{1}{8}} \right)^2 \\
&= (4p+4q+4r-8) \times (6-4\sqrt{2}) + (2pqr - pq - pr - qr + p+q+r-1) \times \left(-\frac{\sqrt{2}}{4} + \frac{3}{8} \right) + 2.
\end{aligned} \tag{39}$$

By applying the definition of IRB for $T_i F_2[p, q, r]$, we have

$$\begin{aligned}
\text{IRB}(T_i F_2[p, q, r]) &= \sum_{uv \in E(T_i F_2[p, q, r])} (\sqrt{d(u)} - \sqrt{d(v)})^2 \\
&= \sum_{uv \in E_1(T_i F_2[p, q, r])} (\sqrt{d(u)} - \sqrt{d(v)})^2 + \sum_{uv \in E_2(T_i F_2[p, q, r])} (\sqrt{d(u)} - \sqrt{d(v)})^2 \\
&\quad + \sum_{uv \in E_3(T_i F_2[p, q, r])} (\sqrt{d(u)} - \sqrt{d(v)})^2 + \sum_{uv \in E_4(T_i F_2[p, q, r])} (\sqrt{d(u)} - \sqrt{d(v)})^2 \\
&= 8 \times (\sqrt{1} - \sqrt{4})^2 + 8(p+q+r-3) \times (\sqrt{2} - \sqrt{4})^2 + (32pqr - 16(pq + pr + qr) \\
&\quad + (8(p+q+r-8)) \times (\sqrt{4} - \sqrt{8})^2 \\
&= (4p+4q+4r-8) \times (48-32\sqrt{2}) + (2pqr - pq - pr - qr + p+q+r-1) \times (12-8\sqrt{2}) + 8.
\end{aligned} \tag{40}$$

By applying the definition of IRDIF for $T_i F_2[p, q, r]$, we have

$$\begin{aligned}
\text{IRDIF}(T_iF_2[p, q, r]) &= \sum_{uv \in E(T_iF_2[p, q, r])} \left| \frac{d(u)}{d(v)} - \frac{d(v)}{d(u)} \right| \\
&= \sum_{uv \in E_1(T_iF_2[p, q, r])} \left| \frac{d(u)}{d(v)} - \frac{d(v)}{d(u)} \right| + \sum_{uv \in E_2(T_iF_2[p, q, r])} \left| \frac{d(u)}{d(v)} - \frac{d(v)}{d(u)} \right| + \sum_{uv \in E_3(T_iF_2[p, q, r])} \left| \frac{d(u)}{d(v)} - \frac{d(v)}{d(u)} \right| \\
&\quad + \sum_{uv \in E_4(T_iF_2[p, q, r])} \left| \frac{d(u)}{d(v)} - \frac{d(v)}{d(u)} \right| \\
&= 8 \times \left| \frac{1}{4} - \frac{4}{1} \right| + 8(p + q + r - 3) \times \left| \frac{2}{4} - \frac{4}{2} \right| + (32pqr - 16(pq + pr + (p + qqr))) + (8 + r - 8) \times \left| \frac{4}{8} - \frac{8}{4} \right| \\
&= 48pqr - 24qr - 24pq - 24pr + 24p + 24q + 24r - 18.
\end{aligned} \tag{41}$$

Theorem 8. Let $T_iF_2[p, q, r]$ be the crystallographic structure of titanium difluoride. Then, the irregularity indices of $T_iF_2[p, q, r]$ are

$$\begin{aligned}
\text{IRLU}(T_iF_2[p, q, r]) &= 32pqr - 16qr - 16pq - 16pr \\
&\quad + 16p + 16q + 16r - 8,
\end{aligned} \tag{42}$$

$$\begin{aligned}
\text{IRLA}(T_iF_2[p, q, r]) &= \frac{32pqr}{3} - \frac{16qr}{3} - \frac{16pq}{3} - \frac{16pr}{3} \\
&\quad + \frac{16p}{3} + \frac{16q}{3} + \frac{16r}{3} - 8,
\end{aligned} \tag{43}$$

$$\begin{aligned}
\text{IRLF}(T_iF_2[p, q, r]) &= (p + q + r - 3) \times 4\sqrt{2} \\
&\quad + (16pqr - 8pq - 8pr - 8qr + 4p \\
&\quad + 4q + 4r - 4) \times \sqrt{2} + 4\sqrt{2}.
\end{aligned} \tag{44}$$

Proof. By applying the definition of IRLU for $T_iF_2[p, q, r]$, we have

$$\begin{aligned}
\text{IRLU}(T_iF_2[p, q, r]) &= \sum_{uv \in E(T_iF_2[p, q, r])} \frac{|d(u) - d(v)|}{\min(d(u), d(v))} \\
&= \sum_{uv \in E_1(T_iF_2[p, q, r])} \frac{|d(u) - d(v)|}{\min(d(u), d(v))} + \sum_{uv \in E_2(T_iF_2[p, q, r])} \frac{|d(u) - d(v)|}{\min(d(u), d(v))} + \sum_{uv \in E_3(T_iF_2[p, q, r])} \frac{|d(u) - d(v)|}{\min(d(u), d(v))} \\
&\quad + \sum_{uv \in E_4(T_iF_2[p, q, r])} \frac{|d(u) - d(v)|}{\min(d(u), d(v))} \\
&= 8 \times \frac{|1 - 4|}{\min(1, 4)} + 8(p + q + r - 3) \times \frac{|2 - 4|}{\min(2, 4)} + (32pqr - 16(pq + pr + (p + qqr))) \\
&\quad + (8 + r - 8) \times \frac{|4 - 8|}{\min(4, 8)} \\
&= 32pqr - 16qr - 16pq - 16pr + 16p + 16q + 16r - 8,
\end{aligned} \tag{45}$$

which is the required result (42). By applying the definition of IRLA for $T_iF_2[p, q, r]$, we have

TABLE 2: Comparison of IRR, IRR_t, and IRF for crystallographic structure Cu₂O[p, q, r].

[p, q, r]	IRR	IRR _t	IRF
[1, 1, 1]	12	6	20
[2, 2, 2]	88	44	160
[3, 3, 3]	308	154	588
[4, 4, 4]	768	384	1496

TABLE 3: Comparison of IRL, IRD₁, and IRGA for crystallographic structure Cu₂O[p, q, r].

[p, q, r]	IRL	IRD ₁	IRGA
[1, 1, 1]	5.5451774444792	7.167037876912	0.4711321426255
[2, 2, 2]	36.0436533891148	50.64039728101	3.062358927066
[3, 3, 3]	116.4487263340632	173.2138414692112	9.8937749951362
[4, 4, 4]	280.0314609461996	427.6207602975844	23.7921732025895

$$\begin{aligned}
\text{IRLA}(T_i F_2[p, q, r]) &= \sum_{uv \in E(T_i F_2[p, q, r])} 2 \frac{|d(u) - d(v)|}{(d(u) + d(v))} \\
&= \sum_{uv \in E_1(T_i F_2[p, q, r])} 2 \frac{|d(u) - d(v)|}{(d(u) + d(v))} + \sum_{uv \in E_2(T_i F_2[p, q, r])} 2 \frac{|d(u) - d(v)|}{(d(u) + d(v))} + \sum_{uv \in E_3(T_i F_2[p, q, r])} 2 \frac{|d(u) - d(v)|}{(d(u) + d(v))} \\
&\quad + \sum_{uv \in E_4(T_i F_2[p, q, r])} 2 \frac{|d(u) - d(v)|}{(d(u) + d(v))} \\
&= 8 \times \frac{|1 - 2|}{(1 + 2)} + 8(p + q + r - 3) \times \frac{|2 - 4|}{(2 + 4)} + (32pqr - 16(pq + pr + (p + qqr) + (8 + r - 8) \times \frac{|4 - 8|}{(4 + 8)} \\
&= \frac{32pqr}{3} - \frac{16qr}{3} - \frac{16pq}{3} - \frac{16pr}{3} + \frac{16p}{3} + \frac{16q}{3} + \frac{16r}{3} - 8,
\end{aligned} \tag{46}$$

which is the required result (43).

By applying the definition of IRLF for $T_i F_2[p, q, r]$, we have

$$\begin{aligned}
\text{IRLF}(T_i F_2[p, q, r]) &= \sum_{uv \in E(T_i F_2[p, q, r])} \frac{|d(u) - d(v)|}{\sqrt{d(u) \times d(v)}} \\
&= \sum_{uv \in E_1(T_i F_2[p, q, r])} \frac{|d(u) - d(v)|}{\sqrt{d(u) \times d(v)}} + \sum_{uv \in E_2(T_i F_2[p, q, r])} \frac{|d(u) - d(v)|}{\sqrt{d(u) \times d(v)}} + \sum_{uv \in E_3(T_i F_2[p, q, r])} \frac{|d(u) - d(v)|}{\sqrt{d(u) \times d(v)}} \\
&\quad + \sum_{uv \in E_4(T_i F_2[p, q, r])} \frac{|d(u) - d(v)|}{\sqrt{d(u) \times d(v)}} \\
&= 8 \times \frac{|1 - 2|}{\sqrt{1 \times 2}} + 8(p + q + r - 3) \times \frac{|2 - 4|}{\sqrt{2 \times 4}} + (32pqr - 16(pq + pr + (p + qqr) + (8 + r - 8) \times \frac{|4 - 8|}{\sqrt{4 \times 8}} \\
&= (p + q + r - 3) \times 4\sqrt{2} + (16pqr - 8pq - 8pr - 8qr + 4p + 4q + 4r - 4) \times \sqrt{2} + 4\sqrt{2},
\end{aligned} \tag{47}$$

TABLE 4: Comparison of IRA, IRB, and IRDIF for crystallographic structure $\text{Cu}_2\text{O}[p, q, r]$.

$[p, q, r]$	IRA	IRB	IRDIF
[1, 1, 1]	0.5147186257614	2.0588745030457	12
[2, 2, 2]	2.9167388793148	15.0984130223353	78
[3, 3, 3]	10.4659453904824	52.8444455781734	252
[4, 4, 4]	17.6720061511424	131.7679681949257	606

TABLE 5: Comparison of IRLU, IRLA, and IRLF for crystallographic structure $\text{Cu}_2\text{O}[p, q, r]$.

$[p, q, r]$	IRLU	IRLA	IRLF
[1, 1, 1]	8	2.0588745030457	16.9705627484771
[2, 2, 2]	52	17.3333333333333	124.4507934888324
[3, 3, 3]	168	56	435.5777772109133
[4, 4, 4]	404	34.6666666666667	1086.1160159025371

TABLE 6: Comparison of IRR, IRR_t , and IRF for crystallographic structure of titanium difluoride $T_iF_2[p, q, r]$.

$[p, q, r]$	IRR	IRR_t	IRF
[1, 1, 1]	24	12	72
[2, 2, 2]	488	244	1832
[3, 3, 3]	2104	1052	8200
[4, 4, 4]	5640	2820	22248

TABLE 7: Comparison of IRL, IRD_1 , and IRGA for the crystallographic structure of titanium difluoride $T_iF_2[p, q, r]$.

$[p, q, r]$	IRL	IRD_1	IRGA
[2, 2, 2]	83.1776616671888	165.8345663143578	69.554205551518
[3, 3, 3]	363.2091226133884	598.8277711408108	440.3809984072711
[4, 4, 4]	975.95123022834	1511.8209759672638	1291.2077912630243

TABLE 8: Comparison of IRA, IRB, and IRDIF for the crystallographic structure of titanium difluoride $T_iF_2[p, q, r]$.

$[p, q, r]$	IRA	IRB	IRDIF
[1, 1, 1]	3.3940296114372	19.6669555172591	12
[2, 2, 2]	7.6833514927824	58.0992795741124	78
[3, 3, 3]	12.3587123434488	108.8848506492402	252
[4, 4, 4]	17.6774714763168	180.259166754825	

TABLE 9: Comparison of IRLU, IRLA, and IRLF for the crystallographic structure of titanium difluoride $T_iF_2[p, q, r]$.

$[p, q, r]$	IRLU	IRLA	IRLF
[1, 1, 1]	24	2.6666666666667	0
[2, 2, 2]	152	45.3333333333333	90.5096679918781
[3, 3, 3]	568	184	84.6660889654819
[4, 4, 4]	1464	482.6666666666667	1018.2337649086285

which is the required formula result (44).

Finally, the next example represents some values of the calculated irregularity indices of $\text{IRLU}(T_iF_2[p, q, r])$,

$\text{IRLA}(T_iF_2[p, q, r])$, $\text{IRLF}(T_iF_2[p, q, r])$, and $\text{IRDIF}(T_iF_2[p, q, r])$ for some test values of $p = 4, q = 1$, and $r = 2$. $\square$

FIGURE 6: Comparison of IRR, IRR_t, and IRF of crystallographic structure Cu₂O[p, q, r].

FIGURE 7: Comparison of IRL, IRD₁, and IRGA for crystallographic structure Cu₂O[p, q, r].

FIGURE 8: Comparison of IRA, IRB, and IRDIF for crystallographic structure Cu₂O[p, q, r].

FIGURE 9: Comparison of IRLU, IRLA, and IRLF for crystallographic structure $\text{Cu}_2\text{O}[p, q, r]$. FIGURE 10: Comparison of IRR, IRR_t , and IRF for crystallographic structure of titanium difluoride $\text{TiF}_2[p, q, r]$. FIGURE 11: Comparison of IRL, IRD_1 , and IRGA for crystallographic structure of titanium difluoride $\text{TiF}_2[p, q, r]$.

FIGURE 12: Comparison of IRA, IRB, and IRDIF for crystallographic structure of titanium difluoride $T_iF_2[p, q, r]$.

FIGURE 13: Comparison of IRLU, IRLA, and IRLF for crystallographic structure of titanium difluoride $T_iF_2[p, q, r]$.

FIGURE 14: The comparison of all irregularity indices for crystallographic structure $Cu_2O[p, q, r]$.

FIGURE 15: The comparison of all irregularity indices for crystallographic structure of titanium difluoride $TiF_2[p, q, r]$.

Example 4. Let $TiF_2[4, 1, 2]$ be the crystallographic structure of titanium difluoride in Figure 5. Then,

$$\begin{aligned} \text{IRLU}(TiF_2[4, 1, 2]) &= 136, \\ \text{IRLA}(TiF_2[4, 1, 2]) &= 40, \\ \text{IRLF}(TiF_2[4, 1, 2]) &= 84.8528137423857, \\ \text{IRDIF}(TiF_2[4, 1, 2]) &= 294. \end{aligned} \quad (48)$$

4. Comparisons and Discussion

The main motivation comes from the fact that graphs of the irregularity indices show close accurate results about properties like entropy, standard enthalpy, vaporization, and acentric factors of octane isomers [8]. Irregularity indices may help to measure the chemical, biological, and nano properties which are widely popular in developing areas.

Through the means of a graph structural analysis and derivation, we compute some irregularity measures of crystallographic structure of molecules $Cu_2O[p, q, r]$ and the crystallographic structure of titanium difluoride of $TiF_2[p, q, r]$. Similar works have been done in [12, 13, 17]. From Tables 2–9, we can easily see that all indices are in increasing order as the values of p, q , and r . On the other hand, indices showed higher values for $Cu_2O[p, q, r]$ and $TiF_2[p, q, r]$. The graphical representations of irregularity indices of $Cu_2O[p, q, r]$ and $TiF_2[p, q, r]$ are depicted in Figures 6–13 for certain values of p, q , and r . Moreover, we presented the comparison of all irregularity indices in Figures 14 and 15 for $Cu_2O[p, q, r]$ and $TiF_2[p, q, r]$, respectively.

5. Conclusion

In this paper, we studied popular crystallographic structure of molecules and also applied analytical methods to compute the irregularity measures for crystallographic structure of molecules $Cu_2O[p, q, r]$ and crystallographic structure of titanium difluoride of $TiF_2[p, q, r]$.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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