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# Investigating Banhatti indices on the molecular graph and the line graph of Glass with M-polynomial approach

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**Abstract**

*Topological indices are numerical values related to a chemical structure that describes the correlation of chemical structure with different physical properties and chemical reactions. Glass has wide applications in architecture, tableware, optics, and optoelectronics.*
*In this article, first, the mathematical relationship between M-polynomial and Banhatti indices such as K-Banhatti, δ-Banhatti, and hyper δ-Banhatti indices are obtained. Then using M-polynomial, Banhatti indices are obtained.*

**Keywords:** *Glass, Topological indices, M-polynomial, Molecular graph, Line graph, Banhatti indices.*

**MSC (2020):** *05C90, 92E10, 05C07, 92E20, 82D80.*

## 1. Introduction

The main application of topological indices in the chemical sciences is the calculation of physical and chemical properties for molecular graphs. For this reason, the theory of chemical graphs is effective in the development of chemical sciences. Amorphous substances may be solid (Glass) or liquid (smelting). Glass is often produced by cooling the melt under its glass transition temperature quickly enough to prevent the formation of crystal phases [22]. For the first time in Germany, the word " glesum " meaning "transparent," was used, from which the word "Glass" was derived [4]. Glass is one of the oldest artificial materials, and today, it has become a tool for decorating architecture and structures (Figure 1.1).

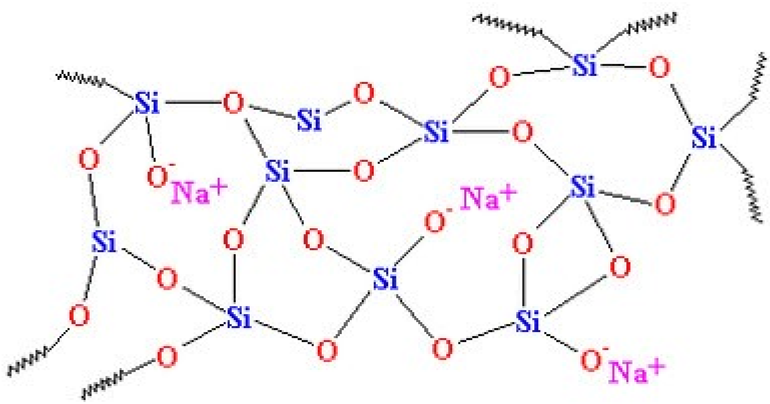


Figure 1.1: Chemical structure of Glass.

Glass can be produced by various methods such as melting hardening [22], physical vapor deposition [2], solid-state reactions (thermochemical methods [24] and chemical mechanics [24]), liquid state reactions (sol-gel process [1,8]), irradiation of crystalline solids (radiative amorphization [21,23]) and under the action of high pressures (pressure amorphism [5,17]). Glass is an amorphous non-crystalline solid and often transparent that has wide applications in architecture, tableware, optics, and optoelectronics.
Topological indices are used to investigate physical and chemical properties in the prediction of the bioactivity of chemical molecules. To further explore these properties, the following sources can be used [9,20].
A significant topological index introduced is the first Zagreb index [7]. In

graph H= (V, E), the first and second Zagreb index are defined as follows:

$$M_1(H) = \sum_{rs\in E(H)} [d_H(r) + d_H(s)], \quad M_2(H) = \sum_{rs\in E(H)} d_H(r)d_H(s),$$

In which the degree of vertex r is indicated by $d_r$.

**Definition 1.** *The first and second K-Banhatti indices in Graph H are defined in the following way [13]:*

$$B_1(H) = \sum_{re} [d_H(r) + d_H(e)], \; B_2(H) = \sum_{re} d_H(r)d_H(e),$$

*Where re means that vertex r and edge e are incidents in H.*

Kulli Calculated the K-Banhatti indices of various chemical networks such as silicate networks, chain silicates, oxides, and honeycomb networks [11]. The K-Banhatti index has also been used to find new drugs and vaccines to prevent the treatment of Covid-19 [12]. The first and second K-Banhatti indices and the first and second K-hyper Banhatti indices of windmill graphs have also been studied [15].
The minimum and maximum vertex degree of graph H denotes by $\delta(H)$ and $\Delta(H)$ respectively. Recently, the conceptual d-vertex degree in chemistry graph theory is defined by Kulli as [14]:

$$\delta_r = d_H(r) - \delta(H) + 1.$$

**Definition 2.** *The first and second $\delta$-Banhatti indices of a graph H are defined as follows [14]:*

$$\delta B_1(H) = \sum_{rs\in E(H)} (\delta_r + \delta_s),$$
$$\delta B_2(H) = \sum_{rs\in E(H)} (\delta_r \delta_s).$$

**Definition 3.** *The first and second hyper d-Banhatti indices of a graph H are defined as follows [14]*

$$H\delta B_1(H) = \sum_{rs\in E(H)} (\delta_r + \delta_s)^2,$$
$$H\delta B_2(H) = \sum_{rs\in E(H)} (\delta_r \delta_s)^2.$$

**Definition 4.** *The M-Polynomial in graph H is defined as [3]:*

$$M(H;x,y) = \sum_{\delta \le i \le j \le \Delta} m_{ij}(H) x^i y^j.$$

*Where* $m_{ij}(H)$ *is the number of edges* $rs \in E(H)$ *such that* $d_r = i$ *and* $d_s = j$.

Some operators, which are used further, are defined as

$$D_x M(H;x,y) = x \times \frac{\partial M(H;x,y)}{\partial x}, \; D_y M(H;x,y) = y \times \frac{\partial M(H;x,y)}{\partial y},$$
$$Q_{x(\alpha)} M(H;x,y) = x^{\alpha} M(H;x,y), \; Q_{y(\alpha)} M(H;x,y) = y^{\alpha} M(H;x,y).$$

One of the applications of the M-Polynomial is that it is possible to calculate topological indices with the help of mathematical relations (derivatives, integrals, etc.) for x and y. The calculation of topological indices using M-polynomial in the molecular graphs has also been investigated [6,19].

**Definition 5.** *In a non-empty graph H, if each edge is considered as a vertex and the two vertices are connected, if the corresponding edges of the two vertices are adjacent to H, the resulting graph is denoted by L(H) and is called the line graph of H [16].*
*In this article, the relationship of M-polynomials with Banhatti indices is studied and Banhatti indices for line graph and molecular graph of Glass are calculated using M-polynomials.*

## 2. Main results

Figure 2.1 shows the Glass's molecular graph.

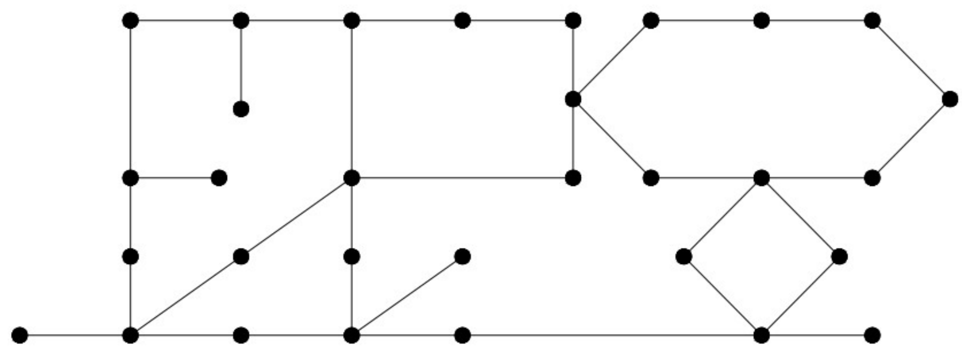

Figure 2.1: The molecular graph of Glass.

The molecular graph of glass is denoted by H. There are seven types of edges in the molecular graph of Glass as follows:

$$\begin{aligned}
E_1 &= \{(d_H(r), d_H(s))\,|rs \in E(H), d_H(r) = 1, d_H(s) = 3\},\\
E_2 &= \{(d_H(r), d_H(s))\,|rs \in E(H), d_H(r) = 1, d_H(s) = 4\},\\
E_3 &= \{(d_H(r), d_H(s))\,|rs \in E(H), d_H(r) = 2, d_H(s) = 2\}\ ,\\
E_4 &= \{(d_H(r), d_H(s))\,|rs \in E(H), d_H(r) = 2, d_H(s) = 3\},\\
E_5 &= \{(d_H(r), d_H(s))\,|rs \in E(H), d_H(r) = 2, d_H(s) = 4\}\ ,\\
E_6 &= \{(d_H(r), d_H(s))\,|rs \in E(H), d_H(r) = 3, d_H(s) = 3\},\\
E_7 &= \{(d_H(r), d_H(s))\,|rs \in E(H), d_H(r) = 3, d_H(s) = 4\}.
\end{aligned}$$

According to Figure 2.1, we have the following table for the molecular graph of Glass:

| Edge type | Number of edges | $d_H(r) + d_H(s)$ | $d_H(r).d_H(s)$ |
|---|---|---|---|
| $E_1$ | 2 | 4 | 3 |
| $E_2$ | 3 | 5 | 4 |
| $E_3$ | 5 | 4 | 4 |
| $E_4$ | 4 | 5 | 6 |
| $E_5$ | 20 | 6 | 8 |
| $E_6$ | 1 | 6 | 9 |
| $E_7$ | 1 | 7 | 12 |

Table 2.1: The number of edges in the molecular graph of Glass.

As a result, the number of edges in the molecular graph of Glass is equal to:

$$|E(H)| = 2 + 3 + 5 + 4 + 20 + 1 + 1 = 36.$$

Figure 2.2 shows the line graph of Glass.

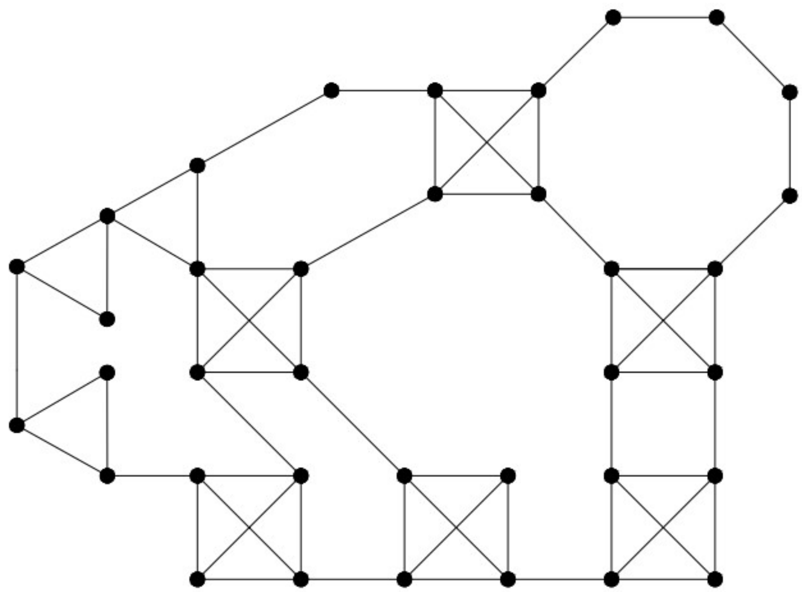

Figure 2.2: The line graph of Glass.

The line graph of glass is denoted by L(H). There are eight types of edges in the line graph of Glass as follows:

$$\begin{aligned}
E'_1 &= \{(d_H(r), d_H(s))\,|rs \in E(L(H)), d_H(r) = 2, d_H(s) = 2\}, \\
E'_2 &= \{(d_H(r), d_H(s))\,|rs \in E(L(H)), d_H(r) = 2, d_H(s) = 3\}, \\
E'_3 &= \{(d_H(r), d_H(s))\,|rs \in E(L(H)), d_H(r) = 2, d_H(s) = 4\}, \\
E'_4 &= \{(d_H(r), d_H(s))\,|rs \in E(L(H)), d_H(r) = 3, d_H(s) = 3\}, \\
E'_5 &= \{(d_H(r), d_H(s))\,|rs \in E(L(H)), d_H(r) = 3, d_H(s) = 4\}, \\
E'_6 &= \{(d_H(r), d_H(s))\,|rs \in E(L(H)), d_H(r) = 3, d_H(s) = 5\}, \\
E'_7 &= \{(d_H(r), d_H(s))\,|rs \in E(L(H)), d_H(r) = 4, d_H(s) = 4\}, \\
E'_8 &= \{(d_H(r), d_H(s))\,|rs \in E(L(H)), d_H(r) = 4, d_H(s) = 5\}.
\end{aligned}$$

According to Figure 2.2, we have the following table for the molecular graph of Glass:

As a result, the number of edges in the line graph of Glass is equal to:

$$|E(L(H))| = 3 + 4 + 4 + 2 + 12 + 1 + 32 + 4 = 62.$$

**Theorem 1.** *Let H= (V, E) be a graph of size m. Then, the following relationships are established between the $\delta B_1(H)$ and $\delta B_2(H)$ index and the first and second Zagreb index:*

$$i)\ \delta B_1(H) = M_1(H) - 2(\delta(H)+1)m\ ,$$
$$ii)\ \delta B_2(H) = M_1(H) + M_2(H) - (\delta(H)-1)^2 m\ .$$

**Proof.**

$$i)\delta B_1(H) = \sum_{rs\in E(H)} (\delta_r + \delta_s\ ) = \sum_{rs\in E(H)} ((d_H(r) - \delta(H)+1)+(d_H(s) - \delta(H)+1))$$
$$= \sum_{rs\in E(H)} ((d_H(r) + d_H(s)) - 2(\delta(H)+1)) = M_1(H) - 2(\delta(H)+1)m,$$

$$ii)\delta B_2(H) = \sum_{rs\in E(H)} (\delta_r.\delta_s\ ) = \sum_{rs\in E(H)} ((d_H(r) - \delta(H)+1).(d_H(s) - \delta(H)+1))$$
$$= \sum_{rs\in E(H)} ((d_H(r)d_H(s)) + (d_H(r) + d_H(s)) + (\delta(H)-1)^2)$$
$$= M_1(H) + M_2(H) + (\delta(H)-1)^2 m.$$

□

**Theorem 2.** *Let $M(H;x,y)$ be the M-Polynomial for the graph H. Then the first K-Banhatti index is computed as,*

$$KB_1(H) = 2D_x + 3D_y + D_x Q_{x(-4)} M\,(H;x,y)\Big|_{(x,y)=(1,1)}\ .$$

| Edge type | Number of edges | $d_H(r) + d_H(s)$ | $d_H(r).d_H(s)$ |
|---|---|---|---|
| $E_1^{'}$ | 3 | 4 | 4 |
| $E_2^{'}$ | 4 | 5 | 6 |
| $E_3^{'}$ | 4 | 6 | 8 |
| $E_4^{'}$ | 2 | 6 | 9 |
| $E_5^{'}$ | 12 | 7 | 12 |
| $E_6^{'}$ | 1 | 8 | 15 |
| $E_7^{'}$ | 32 | 8 | 16 |
| $E_8^{'}$ | 4 | 9 | 20 |

Table 2.2: The number of edges in the line graph of Glass.

**Proof.** According to definitions def1 and def4, the following relations are obtained:

$$\begin{aligned} KB_1(H) = \sum_{re}[d_H(r)+d_H(e)] &= \sum_{rs\in E(H)} (d_H(r)+d_H(e)) + (d_H(s)+d_H(e)) \\ &= \sum_{rs\in E(H)} (d_H(r)+d_H(s)+2d_H(e)) \\ &= \sum_{rs\in E(H)} (d_H(r)+d_H(s)+2(d_H(r)+d_H(s)-2)) \\ &= \sum_{rs\in E(H)} (3d_H(r)+3d_H(s)-4), \end{aligned}$$

$$\begin{aligned} &(D_xQ_{x(-4)})M(H;x,y) = D_xQ_{x(-4)} \sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j \\ &= \sum_{\delta\le i\le j\le\Delta} (i-4)m_{ij}(H)x^{i-4}y^j, \\ &(2D_x)M(H;x,y) = 2D_x \sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j = \sum_{\delta\le i\le j\le\Delta} (2i)m_{ij}(H)x^iy^j, \\ &(3D_y)M(H;x,y) = 3D_y \sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j = \sum_{\delta\le i\le j\le\Delta} (3j)m_{ij}(H)x^iy^j, \\ &(2D_x+3D_y+D_xQ_{x(-4)})M(H;x,y) = \sum_{\delta\le i\le j\le\Delta} (2i+3j+i-4)m_{ij}(H)x^iy^j, \\ &\qquad = \sum_{\delta\le i\le j\le\Delta} (3i+3j-4)m_{ij}(H)x^iy^j. \\ &(2D_x+3D_y+D_xQ_{x(-4)})M(H;x,y)\Big|_{(x,y)=(1,1)} = \sum_{\delta\le i\le j\le\Delta} (3i+3j-4)m_{ij}(H) \\ &\qquad = \sum_{rs\in E(H)} (3d_H(r)+3d_H(s)-4). \end{aligned}$$

Hence,

$$\begin{aligned} &KB_1(H) = (2D_x+3D_y+D_xQ_{x(-4)})M(H;x,y)\Big|_{(x,y)=(1,1)} \\ &= \sum_{rs\in E(H)} 3d_H(r)+3d_H(s)-4. \end{aligned}$$

□

**Theorem 3.** *Let $M(H;x,y)$ be the M-Polynomial for the graph H. Then, the second K-Banhatti index is computed as,*

$$KB_2(H) = ({D_x}^2+{D_y}^2+2D_xD_y-2(D_x+D_y))M(H;x,y)\Big|_{(x,y)=(1,1)}.$$

According to definitions def1 and def4, the following relations are obtained:

$$KB_2(H) = \sum_{re}[d_H(u).d_H(e)] = \sum_{rs\in E(H)}(d_H(r).d_H(e)) + (d_H(s).d_H(e))$$
$$= \sum_{rs\in E(H)} d_G(e)(d_H(r)+d_H(s))$$
$$= \sum_{rs\in E(H)} (d_H(r)+d_H(s)-2)(d_H(r)+d_H(s))$$
$$= \sum_{rs\in E(H)} d_H(r)^2 + d_H(s)^2 + 2(d_H(r).d_H(s)) - 2(d_H(r)+d_H(s)),$$

$$({D_x}^2)M\,(H;x,y) = {D_x}^2 \sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j = \sum_{\delta\le i\le j\le\Delta}(i^2)m_{ij}(H)x^iy^j,$$

$$({D_y}^2)M\,(H;x,y) = {D_y}^2 \sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j = \sum_{\delta\le i\le j\le\Delta}(j^2)m_{ij}(H)x^iy^j,$$

$$2(D_xD_y)M\,(H;x,y) = 2(D_xD_y) \sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j = \sum_{\delta\le i\le j\le\Delta}(2ij)m_{ij}(H)x^iy^j,$$

$$2(D_xD_y)M\,(H;x,y) = 2(D_xD_y) \sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j = \sum_{\delta\le i\le j\le\Delta}(2ij)m_{ij}(H)x^iy^j,$$

$$({D_x}^2+{D_y}^2+2D_xD_y-2(D_x+D_y))M\,(H;x,y)\Big|_{(x,y)=(1,1)}$$
$$= \sum_{\delta\le i\le j\le\Delta}(i^2+j^2+2ij-2(i+j)m_{ij}(H)$$
$$= \sum_{rs\in E(H)} d_H(r)^2 + d_H(s)^2 + 2(d_H(r).d_H(s)) - 2(d_H(r)+d_H(s)),$$

Hence:

$$KB_2(H) = ({D_x}^2+{D_y}^2+2D_xD_y-2(D_x+D_y))M\,(H;x,y)\Big|_{(x,y)=(1,1)}$$
$$= \sum_{rs\in E(H)} d_H(r)^2 + d_H(s)^2 + 2(d_H(r).d_H(s)) - 2(d_H(r)+d_H(s)).$$

**Theorem 4.** *Let $M(H;x,y)$ be the M-Polynomial for the graph $H$. Then, the first $\delta-$ Banhatti index is computed as,*

$$\delta B_1(H) = (D_x+D_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\,(H;x,y)\Big|_{(x,y)=(1,1)}\ .$$

**Proof.** According to definitions def2 and def4, the following relations are obtained:

$$\begin{aligned}\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right) &= \left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)\sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j\\ &= \sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^{i-\delta+1}y^{j-\delta+1},\end{aligned}$$

$$\begin{aligned}&(D_x+D_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right)\\ &=(D_x+D_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)\sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j\\ &=\sum_{\delta\le i\le j\le\Delta}[(i-\delta+1)+(j-\delta+1)]m_{ij}(H)x^{i-\delta+1}y^{j-\delta+1},\end{aligned}$$

$$\begin{aligned}&(D_x+D_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right)\Big|_{(x,y)=(1,1)}\\ &=\sum_{\delta\le i\le j\le\Delta}(i-\delta+1)+(j-\delta+1)m_{ij}(H)\\ &=\sum_{rs\in E(H)}(d_H(r)-\delta+1)+(d_H(s)-\delta+1).\end{aligned}$$

Hence:

$$\delta B_1(H)=(D_x+D_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right)\Big|_{x=y)=1}=\sum_{rs\in E(H)}\delta_r+\delta_s.$$

□

**Theorem 5.** *Let $M(H;x,y)$ be the M-Polynomial for the graph H. Then, the second $\delta-$ Banhatti index is computed as,*

$$\delta B_2(H)=(D_xD_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right)\Big|_{(x,y)=(1,1)}.$$

**Proof.** According to definitions def2 and def4, the following relations are obtained:

$$\begin{aligned}\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right) &= \left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)\sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j\\ &= \sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^{i-\delta+1}y^{j-\delta+1},\end{aligned}$$

$$
\begin{aligned}
&(D_xD_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right)\\
&=(D_xD_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)\sum_{\delta\leq i\leq j\leq\Delta}m_{ij}(H)x^iy^j\\
&=\sum_{\delta\leq i\leq j\leq\Delta}[(i-\delta+1)(j-\delta+1)]m_{ij}(H)x^{i-\delta+1}y^{j-\delta+1},\\
&(D_xD_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right)\Big|_{(x,y)=(1,1)}\\
&=\sum_{\delta\leq i\leq j\leq\Delta}(i-\delta+1)(j-\delta+1)m_{ij}(H)\\
&=\sum_{rs\in E(H)}(d_H(r)-\delta+1)(d_H(s)-\delta+1).
\end{aligned}
$$

Hence:

$$
\delta B_2(H)=(D_xD_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right)\Big|_{(x,y)=(1,1)}=\sum_{rs\in E(H)}\delta_r\delta_s.
$$

□

**Theorem 6.** *Let $M(H;x,y)$ be the M-Polynomial for the graph $H$. Then, the first hyper $\delta-$ Banhatti index is computed as,*

$$
H\delta B_1(H)=({D_x}^2+{D_y}^2+2D_xD_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right)\Big|_{(x,y)=(1,1)}.
$$

**Proof.** According to definitions def3 and def4, the following relations are obtained:

$$
\begin{aligned}
\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right)&=\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)\sum_{\delta\leq i\leq j\leq\Delta}m_{ij}(H)x^iy^j\\
&=\sum_{\delta\leq i\leq j\leq\Delta}m_{ij}(H)x^{i-\delta+1}y^{j-\delta+1},
\end{aligned}
$$

$$
\begin{aligned}
&({D_x}^2+{D_y}^2+2D_xD_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)\sum_{\delta\leq i\leq j\leq\Delta}m_{ij}(H)x^iy^j\\
&=\sum_{\delta\leq i\leq j\leq\Delta}(i-\delta+1)^2m_{ij}(H)x^{i-\delta+1}y^{j-\delta+1}\\
&+\sum_{\delta\leq i\leq j\leq\Delta}(j-\delta+1)^2m_{ij}(H)x^{i-\delta+1}y^{j-\delta+1},\\
&+\sum_{\delta\leq i\leq j\leq\Delta}2(i-\delta+1)(i-\delta+1)m_{ij}(H)x^{i-\delta+1}y^{j-\delta+1}
\end{aligned}
$$

$$
\begin{aligned}
&({D_x}^2+{D_y}^2+2D_xD_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)\sum_{\delta\leq i\leq j\leq\Delta}m_{ij}(H)x^iy^j\Big|_{(x,y)=(1,1)}\\
&\qquad=\sum_{\delta\leq i\leq j\leq\Delta}[(i-\delta+1)^2+(j-\delta+1)^2+2(i-\delta+1)(j-\delta+1)]m_{ij}(H)\\
&\qquad=\sum_{rs\in E(H)}(i-\delta+1)^2+(j-\delta+1)^2+2(i-\delta+1)(j-\delta+1)\\
&\qquad=\sum_{rs\in E(H)}((i-\delta+1)+(j-\delta+1))^2,
\end{aligned}
$$

Hence:

$$H\ \delta B_1(H) = ({D_x}^2 + {D_y}^2 + 2D_xD_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)\sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j\Big|_{(x,y)=(1,1)}$$
$$= \sum_{rs\in E(H)} (\delta_r + \delta_s)^2.$$

□

**Theorem 7.** *Let $M(H;x,y)$ be the M-Polynomial for the graph H. Then, the second hyper $\delta - Banhatti$ index is computed as,*

$$H\delta B_2(H) = ({D_x}^2{D_y}^2)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right)\Big|_{(x,y)=(1,1)}\ .$$

**Proof.** According to definitions def3 and def4, the following relations are obtained:

$$\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M\left(H;x,y\right) = \left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)\sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j$$
$$= \sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^{i-\delta+1}y^{j-\delta+1},$$

$$({D_x}^2{D_y}^2)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)\sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j$$
$$= \sum_{\delta\le i\le j\le\Delta} (i-\delta+1)^2(j-\delta+1)^2 m_{ij}(H)x^{i-\delta+1}y^{j-\delta+1},$$
$$({D_x}^2{D_y}^2)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)\sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j\Big|_{(x,y)=(1,1)}$$
$$= \sum_{\delta\le i\le j\le\Delta} (i-\delta+1)^2(j-\delta+1)^2 m_{ij}(H) = \sum_{rs\in E(H)} (i-\delta+1)^2(j-\delta+1)^2,$$

Hence:

$$H\ \delta B_2(H) = ({D_x}^2{D_y}^2)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)\sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j\Big|_{(x,y)=(1,1)}$$
$$= \sum_{rs\in E(H)} {\delta_r}^2{\delta_s}^2 = \sum_{rs\in E(H)} (\delta_r\delta_s)^2.$$

□

**Theorem 8.** *Let H be the molecular graph of Glass. Then the M-Polynomial of H is as follows,*

$$M(H;\ x,\ y) = 2x^1y^3 + 3x^1y^4 + 5x^2y^2 + 4x^2y^3 + 20x^2y^4 + 1x^3y^3 + 1x^3y^4.$$

**Proof.** According to definitions def4 and Table t1, the following relationships are obtained:

$$\begin{aligned} M(H;x,y) &= \sum_{\delta\le i\le j\le\Delta} m_{ij}(H)x^iy^j = \sum_{rs\in E_1} m_{ij}(H)x^iy^j + \sum_{rs\in E_2} m_{ij}(H)x^iy^j \\ &+ \sum_{rs\in E_3} m_{ij}(H)x^iy^j \\ &+ \sum_{rs\in E_4} m_{ij}(H)x^iy^j + \sum_{rs\in E_5} m_{ij}(H)x^iy^j \\ &+ \sum_{rs\in E_6} m_{ij}(H)x^iy^j + \sum_{rs\in E_7} m_{ij}(H)x^iy^j \\ &= 2x^1y^3 + 2x^1y^4 + 6x^2y^2 + 2x^2y^3 + 18x^2y^4 + 2x^3y^3 + 4x^3y^4. \end{aligned}$$

□

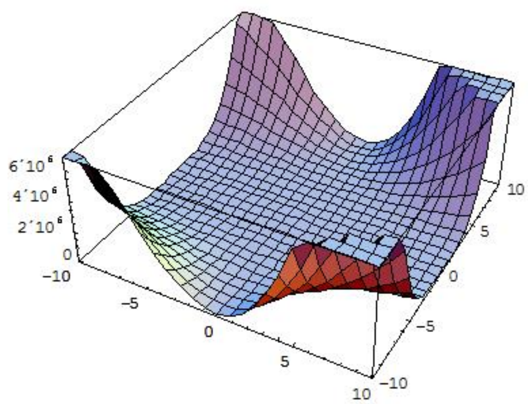


Figure 2.3: M-polynomial of the molecular graph of Glass.

The behavior of M-polynomial in the molecular graph of Glass (Figure 2.3) shows that this M-polynomial is always positive for different values of x and y.

According to the results of the above theorems, table tab2.3 is obtained to calculate Banhatti indices using M-polynomial.

| Topological Index | formula | Derivation from M(H; x, y) |
|---|---|---|
| First K-Banhatti | $\sum_{re}[d_H(r)+d_H(e)]$ | $2D_x+3D_y+D_xQ_{x(-4)}M(H;x,y)\big\|_{x=y=1}$ |
| Second K-Banhatti | $\sum_{re}[d_H(r).d_H(e)]$ | $({D_x}^2+{D_y}^2+2D_xD_y-2(D_x+D_y))M(H;x,y)\big\|_{x=y=1}$ |
| First $\delta$-Banhatti | $\sum_{rs\in E(H)}\delta_r+\delta_s$ | $(D_x+D_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M(H;x,y)\big\|_{x=y=1}$ |
| Second $\delta$-Banhatti | $\sum_{rs\in E(H)}\delta_r.\delta_s$ | $(D_xD_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M(H;x,y)\big\|_{x=y=1}$ |
| First hyper $\delta$-Banhatti | $\sum_{rs\in E(H)}(\delta_r+\delta_s)^2$ | $({D_x}^2+{D_y}^2+2D_xD_y)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M(H;x,y)\big\|_{x=y=1}$ |
| Second hyper $\delta$-Banhatti | $\sum_{rs\in E(H)}(\delta_r.\delta_s)^2$ | $({D_x}^2{D_y}^2)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M(H;x,y)\big\|_{x=y=1}$ |

Table 2.3: Derivation of Banhatti indices from M-polynomial.

**Theorem 9.** *Let $H'$ be the line graph of Glass. Then the M-Polynomial of $H'$ is as follows,*

$$M(H';\,x,\,y)=3x^2y^2+4x^2y^3+4x^2y^4+2x^3y^3+12x^3y^4+1x^3y^5+32x^4y^4+4x^4y^5.$$

**Proof.** According to definitions def4 and Table tab22, the following relationships are obtained:

$$\begin{aligned}
M\left(H';x,y\right) &= \sum_{\delta\le i\le j\le\Delta} m_{ij}(H')x^iy^j\\
&= \sum_{rs\in E_1} m_{ij}(H')x^iy^j + \sum_{rs\in E_2} m_{ij}(H')x^iy^j\\
&+ \sum_{rs\in E_3} m_{ij}(H')x^iy^j + \sum_{rs\in E_4} m_{ij}(H')x^iy^j\\
&+ \sum_{rs\in E_5} m_{ij}(H')x^iy^j + \sum_{rs\in E_6} m_{ij}(H')x^iy^j\\
&+ \sum_{rs\in E_7} m_{ij}(H')x^iy^j + \sum_{rs\in E_8} m_{ij}(H')x^iy^j\\
&= 3x^2y^2+4x^2y^3+4x^2y^4+2x^3y^3+12x^3y^4+x^3y^5+32x^4y^4+4x^4y^5.
\end{aligned}$$

$\square$

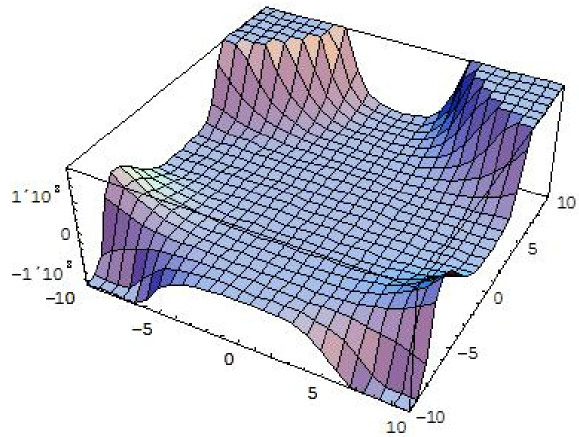


Figure 2.4: M-polynomial of the molecular graph of Glass.

The behavior of M-polynomial in the line graph of Glass (figure 2.4) shows that this M-polynomial is not always positive for different values of x and y, and can be negative for negative values of y.

**Theorem 10.** *Let H be the molecular graph of Glass. Then the Banhatti indices of H are as follows,*

1. $KB_1(H) = 444$,
2. $KB_2(H) = 700$,
3. $\delta B_1(H) = 196$,
4. $\delta B_2(H) = 243$,
5. $H\delta B_1(H) = 1092$,
6. $H\delta B_2(H) = 1795$.

**Proof.** According to Theorem thm2.8, M-polynomial of H is as follows:

$$M(H;\, x,\, y) = 2x^1y^3 + 3x^1y^4 + 5x^2y^2 + 4x^2y^3 + 20x^2y^4 + 1x^3y^3 + 1x^3y^4.$$

□

We know in the molecular graph of Glass $\delta(H) = 1$ and $-\delta + 1 = -1 + 1 = 0$.Then

$$D_x(M(H;x,y)) = 2x^1y^3 + 3x^1y^4 + 10x^2y^2 + 8x^2y^3 + 40x^2y^4 + 3x^3y^3 + 3x^3y^4,$$

$$D_y(M(H;x,y)) = 6x^1y^3 + 12x^1y^4 + 10x^2y^2 + 12x^2y^3 + 80x^2y^4 + 3x^3y^3 + 4x^3y^4,$$

$$D_xD_y(M(H;x,y)) = 6x^1y^3 + 12x^1y^4 + 20x^2y^2 + 24x^2y^3 + 160x^2y^4 + 9x^3y^3 + 12x^3y^4,$$

$(D_x+D_y)(M(H;x,y)) = 8x^1y^3+15x^1y^4+20x^2y^2+20x^2y^3+120x^2y^4+6x^3y^3+7x^3y^4,$

$$Q_{x(-\delta+1)}Q_{y(-\delta+1)}M(H;x,y) = Q_{x(0)}Q_{y(0)}M(H;x,y) \\ = 2x^1y^3+3x^1y^4+5x^2y^2+4x^2y^3+20x^2y^4+1x^3y^3+x^3y^4,$$

$$D_xQ_{x(-4)}M(H;x,y) = -6x^{-3}y^3-9x^{-3}y^4-10x^{-2}y^2-8x^{-2}y^3-40x^{-2}y^4 \\ -x^{-1}y^3-x^{-1}y^4,$$

$D_x^2(M(H;x,y)) = 2x^1y^3+3x^1y^4+20x^2y^2+16x^2y^3+80x^2y^4+9x^3y^3+9x^3y^4,$

${D_y}^2(M(H;x,y)) = 18x^1y^3+48x^1y^4+20x^2y^2+36x^2y^3+320x^2y^4+9x^3y^3+16x^3y^4,$

$${D_x}^2{D_y}^2(M(H;x,y)) = 18x^1y^3+48x^1y^4+80x^2y^2+144x^2y^3+1280x^2y^4 \\ +81x^3y^3+144x^3y^4,$$

Now we have:

$$1. KB_1(H) = 2D_x+3D_y+D_xQ_{x(-4)}M(H;x,y)\Big|_{(x,y)=(1,1)} \\ = 2(2+3+10+8+40+3+3)+3(6+12+10+12+80+3+4) \\ +(-6-9-10-8-40-1-1) \\ = 138+381-75 = 444,$$

$$2.\ KB_2(H) = ({D_x}^2+{D_y}^2+2D_xD_y-2(D_x+D_y))M(H;x,y)\Big|_{(x,y)=(1,1)} \\ = (2+3+20+16+80+9+9)+(18+48+20+36+320+9+16) \\ -2(8+15+20+20+120+6+7)+2(6+12+20+24+160+9+12) \\ = 139+467+486-392 = 700,$$

$$3.\ \delta B_1(H) = (D_x+\ D_y)\left(Q_{x(0)}Q_{y(0)}\right)M(H;x,y)\Big|_{(x,y)=(1,1)} \\ = 8+15+20+20+120+6+7 = 196,$$

$$4.\ \delta B_2(H) = (D_xD_y)\left(Q_{x(0)}Q_{y(0)}\right)M(H;x,y)\Big|_{(x,y)=(1,1)} \\ = 6+12+20+24+160+9+12 = 243,$$

$$5.\ H\delta B_1(H) = ({D_x}^2+{D_y}^2+2D_xD_y)\left(Q_{x(0)}Q_{y(0)}\right)M(H;x,y)\Big|_{(x,y)=(1,1)} \\ = (2+3+20+16+80+9+9)+(18+48+20+36+320+9+16) \\ +2(6+12+20+24+160+9+12), \\ = 139+467+486 = 1092,$$

$$6.\ H\delta B_2(H) = ({D_x}^2{D_y}^2)\left(Q_{x(-\delta+1)}Q_{y(-\delta+1)}\right)M(H;x,y)\Big|_{(x,y)=(1,1)} \\ = ({D_x}^2{D_y}^2)\left(Q_{x(0)}Q_{y(0)}\right)M(H;x,y)\Big|_{(x,y)=(1,1)} \\ = ({D_x}^2{D_y}^2)M(H;x,y)\Big|_{(x,y)=(1,1)} \\ = 18+48+80+144+1280+81+144 = 1795.$$

□

**Theorem 11.** *Let $H^{'}$ be the line graph of Glass. Then the Banhatti indices of $H^{'}$ are as follows,*

1. $KB_1(H') = 1108,$
2. $KB_2(H') = 2484,$
3. $\delta B_1(H') = 576,$
4. $\delta B_2(H') = 1351,$
5. $HB_1(H') = 5444,$
6. $HB_2(H') = 31207.$

**Proof.** According to Theorem thm2.9, M-polynomial of $H^{'}$ is as follows:

$$M(H';\, x,\, y) = 3x^2y^2{+}4x^2y^3{+}4x^2y^4{+}2x^3y^3{+}12x^3y^4{+}1x^3y^5{+}32x^4y^4{+}4x^4y^5.$$

We know in the line graph of Glass $\delta(H^{'}) = 2$ and $-\delta + 1 = -2 + 1 = -1$.
Then

$$D_x(M(H';x,y)) = 6x^2y^2{+}8x^2y^3{+}8x^2y^4{+}6x^3y^3{+}36x^3y^4{+}3x^3y^5{+}128x^4y^4{+}16x^4y^5,$$

$$D_y(M(H';x,y)) = 6x^2y^2{+}12x^2y^3{+}16x^2y^4{+}6x^3y^3{+}48x^3y^4{+}5x^3y^5{+}128x^4y^4{+}20x^4y^5,$$

$$\begin{aligned} D_xD_y(M(H';x,y)) &= 12x^2y^2 + 24x^2y^3 + 32x^2y^4 + 18x^3y^3 + 144x^3y^4 + 15x^3y^5 \\ &+512x^4y^4 + 80x^4y^5, \end{aligned}$$

$$\begin{aligned} (D_x + D_y)(M(H';x,y)) &= 12x^2y^2 + 20x^2y^3 + 24x^2y^4 + 12x^3y^3 + 84x^3y^4 + 8x^3y^5 \\ &+256x^4y^4 + 36x^4y^5, \end{aligned}$$

$$\begin{aligned} Q_{x(-\delta+1)}Q_{y(-\delta+1)}M\left(H';x,y\right) &= Q_{x(1)}Q_{y(1)}M\left(H';x,y\right) \\ &= 3x^3y^3 + 4x^3y^4 + 4x^3y^5 + 2x^4y^4 + 12x^4y^5 + 1x^4y^6 + 32x^5y^5 + 4x^5y^6, \end{aligned}$$

$$D_xQ_{x(-4)}M\left(H';x,y\right) = -6x^{-2}y^2{-}8x^{-2}y^3{-}8x^{-2}y^4{-}2x^{-1}y^3{-}12x^{-1}y^4{-}1x^{-1}y^5,$$

$$\begin{aligned} D_x^2(M(H';x,y)) &= 12x^2y^2 + 16x^2y^3 + 16x^2y^4 + 18x^3y^3 + 108x^3y^4 + 9x^3y^5 \\ &+512x^4y^4 + 64x^4y^5, \\ D_y^2(M(H';x,y)) &= 12x^2y^2 + 36x^2y^3 + 64x^2y^4 + 18x^3y^3 + 192x^3y^4 + 25x^3y^5 \\ &+512x^4y^4 + 100x^4y^5, \\ D_x^2D_y^2(M(H';x,y)) &= 48x^2y^2 + 144x^2y^3 + 256x^2y^4 + 162x^3y^3 + 1728x^3y^4 \\ &+225x^3y^5 + 8192x^4y^4 + 1600x^4y^5, \end{aligned}$$

Now we have:

$$\begin{aligned} &1.KB_1(H') = 2D_x + 3D_y + D_xQ_{x(-4)}M\left(H';x,y\right)\Big|_{(x,y)=(1,1)} \\ &= 2\left(6+8+8+6+36+3+128+16\right) + 3(6+12+16+6+48+5+128+20) \\ &\quad -(6+8+8+2+12+1) = 422 + 723 - 37 = 1108, \end{aligned}$$

2. $KB_2(H') = ({D_x}^2 + {D_y}^2 + 2D_xD_y - 2(D_x + D_y))M\left(H'; x, y\right)\Big|_{(x,y)=(1,1)}$
$= (12 + 16 + 16 + 18 + 108 + 9 + 512 + 64)$
$+(12 + 36 + 64 + 18 + 192 + 25 + 512 + 100)$
$+2(12 + 24 + 32 + 18 + 144 + 15 + 512 + 80)$
$-2(12 + 20 + 24 + 12 + 84 + 8 + 256 + 36) = 755 + 959 + 1674 - 904 = 2484,$

3. $\delta B_1(H') = (D_x + D_y)\left(Q_{x(1)}Q_{y(1)}\right) M\left(H'; x, y\right)\Big|_{(x,y)=(1,1)}$
$= 18 + 28 + 32 + 16 + 108 + 10 + 320 + 44 = 576,$

4. $\delta B_2(H') = (D_xD_y)\left(Q_{x(1)}Q_{y(1)}\right) M\left(H'; x, y\right)\Big|_{(x,y)=(1,1)}$
$= 27 + 48 + 60 + 32 + 240 + 24 + 800 + 120 = 1351,$

5. $H\delta B_1(H') = ({D_x}^2 + {D_y}^2 + 2D_xD_y)\left(Q_{x(1)}Q_{y(1)}\right) M\left(H'; x, y\right)\Big|_{(x,y)=(1,1)}$
$= (27 + 36 + 36 + 32 + 192 + 16 + 800 + 100)$
$+(27 + 64 + 100 + 32 + 300 + 36 + 800 + 144)$
$+2(27 + 48 + 60 + 32 + 240 + 24 + 800 + 120) = 1239 + 1503 + 2702 = 5444,$

6. $H\delta B_2(H') = ({D_x}^2{D_y}^2)\left(Q_{x(1)}Q_{y(1)}\right) M\left(H'; x, y\right)\Big|_{(x,y)=(1,1)}$
$= 243 + 576 + 900 + 512 + 4800 + 576 + 20000 + 3600 = 31207.$

□

## 3. Conclusion

In this article, Banhatti indices of the molecular graph and the line graph of Glass were obtained by mathematical operations on M-polynomial.
The results of calculating the topological indices of Banhatti indices in the molecular graph and the line graph show that these topological indices have smaller values in the molecular graph than in the line graph of Glass. Considering the wide applications of Glass, the calculations of this article can be used in the production of higher quality Glass.

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