



SUPPLEMENTARY MATERIAL TO
**Computation of Zagreb and atom–bond connectivity indices of
certain families of dendrimers by using
automorphism group action**

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CONSIDERATIONS OF ZAGREB GROUP INDICES

It was Randić who presented in 1975 a bond-additive topological index called branching index as a descriptor for describing molecular branching.¹ The Randić index was defined as follows:

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

Later, this index was renamed as connectivity index and generalized to connectivity indices of various orders, such as the zero-*th* order, the first order connectivity index (second Zagreb index) and of higher orders. The families of the Zagreb indices are applied to investigate the complexity of molecules, chirality, *Z/E*-isomerism and hetero-systems. Moreover, the Zagreb indices revealed a probable applicability for developing multi-linear regression models and thus have great importance in QSPR/QSAR modeling. The first and second Zagreb indices of a graph *G* are defined as:

$$M_1(G) = \sum_{v \in U(G)} (d_v)^2 = \sum_{e=uv \in E(G)} (d_u + d_v)$$
$$M_2(G) = \sum_{e=uv \in E(G)} (d_u \times d_v)$$

The first and second Zagreb co-indices of a graph *G* are defined as:

$$\bar{M}_1(G) = \sum_{e=uv \notin E(G)} (d_u + d_v)$$

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$$\bar{M}_2(G) = \sum_{e=uv \notin E(G)} (d_u \times d_v)$$

where d_u and d_v denote the degree of the vertex u and vertex v , respectively.

The first and second Zagreb polynomials for a graph G and in variable x are given as:

$$Zg_1(G, x) = \sum_{e=uv \in E(G)} x^{(d_u+d_v)}$$

$$Zg_2(G, x) = \sum_{e=uv \in E(G)} x^{(d_u \times d_v)}$$

The first and second modified Zagreb indices of a graph G are defined as:

$${}^m M_1(G) = \sum_{v \in U(G)} (d_v)^{-2} = \sum_{e=uv \in E(G)} (d_u + d_v)^{-1}$$

$${}^m M_2(G) = \sum_{e=uv \in E(G)} (d_u \times d_v)^{-1}$$

The first and second variable Zagreb indices of a graph G are defined as:

$${}^v M_1(G) = \sum_{v \in U(G)} (d_v)^{2v} = \sum_{e=uv \in E(G)} (d_u + d_v)^v$$

$${}^v M_2(G) = \sum_{e=uv \in E(G)} (d_u \times d_v)^v$$

for

$$v = 1, \quad {}^v M_r(G) = M_r(G)$$

$$v = -1, \quad {}^v M_r(G) = {}^m M_r(G)$$

and

$$v = \frac{-1}{2}, \quad {}^v M_1(G) = \chi(G)$$

where $r=1, 2$.

In 2013, Shirdel, Rezapour and Sayadi² introduced a distance-based Zagreb index named hyper-Zagreb index that is given by:

$$HM(G) = \sum_{e=uv \in E(G)} (d_u + d_v)^2$$

In the augmented Zagreb index of a graph, G is defined as:³

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u \times d_v}{d_u + d_v - 2} \right)^3$$

Proof for Theorem 1

It is easy to see that $d_{v_{01}} = 2 = d_{v_{02}}, d_{v_{(n+1)0}} = 1$, $d_{v_{it}} = 2 + \delta_{0t}$, where $1 \leq i \leq n$ and $0 \leq t \leq 3$. Now, by using Automorphism group action on the vertices and edges of $G[n]$ and Lemma 1, one obtains:

$$\begin{aligned} M_1(G[n]) &= |I_1| (d_{v_{01}})^2 + |I_2| (d_{v_{02}})^2 + \sum_{i=1}^n \sum_{t=0}^3 |I_{it}| (d_{v_{it}})^2 + 2^{n+1} (d_{v_{(n+1)0}})^2 = \\ &= 17 \times 2^{n+2} - 50, \end{aligned}$$

$$M_2(G[n]) = |S_1| (d_{v_{10}} d_{v_{01}}) + |S_2| (d_{v_{01}} d_{v_{02}}) + |S_3| (d_{v_{02}} d_{v_{03}}) +$$

$$+ \sum_{i=1}^n \sum_{t=1}^3 |M_{it}| (d_{v_{i(t-1)}} d_{v_{it}}) + \sum_{i=1}^n |N_i| (d_{v_{i3}} d_{v_{(i+1)0}}) =$$

$$= 9 \times 2^{n+3} - 56,$$

$$Z_{g_1}(G, x) = \sum_{uv \in E(G)} x^{d_u + d_v} =$$

$$= |S_1| x^{(d_{v_{10}} + d_{v_{01}})} + |S_2| x^{(d_{v_{01}} + d_{v_{02}})} + |S_3| x^{(d_{v_{02}} + d_{v_{03}})} +$$

$$+ \sum_{i=1}^n \sum_{t=1}^3 |M_{it}| x^{(d_{v_{i(t-1)}} + d_{v_{it}})} + \sum_{i=1}^n |N_i| x^{(d_{v_{i3}} + d_{v_{(i+1)0}})} =$$

$$= (3 \times 2^{n+1} - 6)x^5 + (2^{n+3} - 5)x^4 + 2^{n+1}x^3,$$

$$Z_{g_2}(G, x) = \sum_{uv \in E(G)} x^{d_u d_v} =$$

$$= |S_1| x^{(d_{v_{10}} d_{v_{01}})} + |S_2| x^{(d_{v_{01}} d_{v_{02}})} + |S_3| x^{(d_{v_{02}} d_{v_{03}})} +$$

$$+ \sum_{i=1}^n \sum_{t=1}^3 |M_{it}| x^{(d_{v_{i(t-1)}} d_{v_{it}})} + \sum_{i=1}^n |N_i| x^{(d_{v_{i3}} d_{v_{(i+1)0}})} =$$

$$= (3 \times 2^{n+1} - 6)x^6 + (2^{n+3} - 5)x^4 + 2^{n+1}x^2.$$

Proof for Theorem 2

Since in the first and second Zagreb co-indices all those pairs of vertices are considered which are not adjacent with each other, one can write:

$$\bar{M}_1(G[n]) = M_1(K_n) - M_1(G[n]) =$$

$$= n(n-1)^2 - \sum_{i=1}^k |E_i| (d_{x_{j-1}} + d_{x_j}) =$$

$$\begin{aligned}
 &= n(n-1)^2 - [|S_1| (d_{v_{10}} + d_{v_{01}}) + |S_2| (d_{v_{01}} + d_{v_{02}}) + |S_3| (d_{v_{02}} + d_{v_{03}}) \\
 &+ \sum_{i=1}^n \sum_{t=1}^3 |M_{it}| (d_{v_{i(t-1)}} + d_{v_{it}}) + \sum_{i=1}^n |N_i| (d_{v_{i3}} + d_{v_{(i+1)0}})] = \\
 &= (16 \times 2^n - 10)(16 \times 2^n - 11)^2 - (17 \times 2^{n+2} - 50) = \\
 &= (16 \times 2^n - 10)(256 \times 2^{2n} + 121 - 352 \times 2^n) - (17 \times 2^{n+2} - 50) = \\
 &= 4096 \times 2^{3n} - 8192 \times 2^{2n} + 5388 \times 2^n - 1160, \\
 &\bar{M}_2(G[n]) = n(n-1)^2 - \sum_{i=1}^k |E_i| (d_{x_{j-1}} d_{x_j}) = \\
 &= n(n-1)^2 - [|S_1| (d_{v_{10}} d_{v_{01}}) + |S_2| (d_{v_{01}} d_{v_{02}}) + |S_3| (d_{v_{02}} d_{v_{03}}) + \\
 &+ \sum_{i=1}^n \sum_{t=1}^3 |M_{it}| (d_{v_{i(t-1)}} d_{v_{it}}) + \sum_{i=1}^n |N_i| (d_{v_{i3}} d_{v_{(i+1)0}})] = \\
 &= (16 \times 2^n - 10)(16 \times 2^n - 11)^2 - (9 \times 2^{n+3} - 56) = \\
 &= 4096 \times 2^{3n} + 1936 \times 2^n - 5632 \times 2^{2n} - 2560 \times 2^{2n} - \\
 &- 1210 + 3520 \times 2^n - 72 \times 2^n + 56 = \\
 &= 4096 \times 2^{3n} - 8192 \times 2^{2n} + 5384 \times 2^n - 1154,
 \end{aligned}$$

where $n = 16 \times 2^n - 10$.

Proof for Theorem 3

$$\begin{aligned}
 {}^v M_1(G[n]) &= |I_1| (d_{v_{01}})^{2v} + |I_2| (d_{v_{02}})^{2v} + \\
 &+ \sum_{i=1}^n \sum_{t=0}^3 |I_{it}| (d_{v_{it}})^{2v} + 2^{n+1} (d_{v_{(n+1)0}})^{2v} = \\
 &= 2(2^{2v}) + 2(2^{2v}) + \sum_{i=1}^n \sum_{t=0}^3 2^{i+1-\delta_{0t}} (2 + \delta_{0t})^{2v} + 2^{n+1} (1)^{2v} = \\
 &= 4(2)^{2v} + \sum_{i=1}^n (2^i \times 3^{2v} + 2^{i+1} \times 2^{2v} + 2^{i+1} \times 2^{2v} + 2^{i+1} \times 2^{2v}) + 2^{n+1} = \\
 &= 4(2)^{2v} + 2(2^n - 1)(9^v + 6 \times 2^{2v}) + 2^{n+1} = \\
 &= -2\{4 \times 2^{2v} + 3^{2v}\} + 2^{n+1}\{1 + 3^{2v} + 6 \times 2^{2v}\}. \\
 {}^v M_2(G[n]) &= |S_1| (d_{v_{10}} d_{v_{01}})^v + |S_2| (d_{v_{01}} d_{v_{02}})^v + |S_3| (d_{v_{02}} d_{v_{03}})^v + \\
 &+ \sum_{i=1}^n \sum_{t=1}^3 |M_{it}| (d_{v_{i(t-1)}} d_{v_{it}})^v + \sum_{i=1}^n |N_i| (d_{v_{i3}} d_{v_{(i+1)0}})^v =
 \end{aligned}$$

$$\begin{aligned}
&= 2(6)^v + 2(4)^v + (4)^v + \sum_{i=1}^n 2^{i+1}(6^v + 4^v + 4^v) + \sum_{i=1}^{n-1} 2^{i+1}6^v + 2^{n+1}(2)^v = \\
&= 2(6)^v + 3(4)^v + 4(2^n - 1)(6^v + 2 \times 4^v) + 4(2^{n-1} - 1)6^v + 2^{n+1}(2)^v = \\
&= -6 \times 6^h - 5 \times 4^v + 2^{n+1} \{3 \times 6^v + 4 \times 4^v + 2^v\}.
\end{aligned}$$

Proof for Theorem 4

$$\begin{aligned}
HM(G[n]) &= |S_1| (d_{v_{10}} + d_{v_{01}})^2 + |S_2| (d_{v_{01}} + d_{v_{02}})^2 + \\
&+ |S_3| (d_{v_{02}} + d_{v_{03}})^2 + \sum_{i=1}^n \sum_{t=1}^3 |M_{it}| (d_{v_{i(t-1)}} + d_{v_{it}})^2 + \\
&\quad + \sum_{i=1}^n |N_i| (d_{v_{i3}} + d_{v_{(i+1)0}})^2 = \\
&= 98 + 114 \sum_{i=1}^n 2^i + 50 \sum_{i=1}^{n-1} 2^i + 18.2^n = 37 \times 2^{n+3} - 230, \\
AZI(G[n]) &= |S_1| \left(\frac{d_{v_{10}} d_{v_{01}}}{d_{v_{10}} + d_{v_{01}} - 2} \right)^3 + |S_2| \left(\frac{d_{v_{01}} d_{v_{02}}}{d_{v_{01}} + d_{v_{02}} - 2} \right)^3 + \\
&+ |S_3| \left(\frac{d_{v_{02}} d_{v_{03}}}{d_{v_{02}} + d_{v_{03}} - 2} \right)^3 + \sum_{i=1}^n \sum_{t=1}^3 |M_{it}| \left(\frac{d_{v_{i(t-1)}} d_{v_{it}}}{d_{v_{i(t-1)}} + d_{v_{it}}} \right)^3 + \\
&\quad + \sum_{i=1}^n |N_i| \left(\frac{d_{v_{i3}} d_{v_{(i+1)0}}}{d_{v_{i3}} + d_{v_{(i+1)0}} - 2} \right)^3 = \\
&= 2(2)^3 + 2(2)^3 + (2)^3 + \sum_{i=1}^n 2^{i+1} \{ (2)^3 + (2)^3 + (2)^3 \} + \\
&\quad + \sum_{i=1}^{n-1} 2^{i+1} (2)^3 + 2^{n+1} (2)^3 = \\
&= 2^{n+7} - 88.
\end{aligned}$$

Proof for Theorem 5

It is easy to see that $d_{v_{01}} = 2 = d_{v_{02}}$, $d_{v_{(n+1)0}} = 1$ and $d_{v_{it}} = 2 + \delta_{0t}$ where $1 \leq i \leq n$ and $0 \leq t \leq 6$. Now, by using Automorphism group action on the vertices and edges of $H[n]$ and Lemma 1, one obtains:

$$M_1(H[n]) = |I| (d_{v_{01}})^2 + \sum_{i=1}^n \sum_{t=0}^6 |I_{it}| (d_{v_{it}})^2 + 2^{n+1} (d_{v_{(n+1)0}})^2$$

$$\begin{aligned}
 &= 29 \times 2^{n+2} - 106, \\
 M_2(H[n]) &= |S_1|(d_{v_{10}}d_{v_{01}}) + |S_2|(d_{v_{01}}d_{v_{02}}) + \\
 &+ \sum_{i=1}^n \sum_{t=1}^6 |M_{it}|(d_{v_{i(t-1)}}d_{v_{it}}) + \sum_{i=1}^n |N_i|(d_{v_{i6}}d_{v_{(i+1)0}}) = \\
 &= 2(3.2) + (2.2) + \sum_{i=1}^n 2^{i+1} \{ (d_{v_{10}}d_{v_{11}}) + (d_{v_{11}}d_{v_{12}}) + (d_{v_{12}}d_{v_{13}}) + (d_{v_{13}}d_{v_{14}}) + \\
 &+ (d_{v_{14}}d_{v_{15}}) + (d_{v_{15}}d_{v_{16}}) \} + \sum_{i=1}^{n-1} 2^{i+1} (d_{v_{i6}}d_{v_{(i+1)0}}) + 2^{n+1} (d_{v_{n6}}d_{v_{(n+1)0}}) = \\
 &= 15 \times 2^{n+3} - 112, \\
 Z_{g1}(H, x) &= \sum_{uv \in E(G)} x^{d_u + d_v} = \\
 &= |S_1| x^{(d_{v_{10}} + d_{v_{01}})} + |S_2| x^{(d_{v_{01}} + d_{v_{02}})} + \sum_{i=1}^n \sum_{t=1}^6 |M_{it}| x^{(d_{v_{i(t-1)}} + d_{v_{it}})} + \\
 &+ \sum_{i=1}^n |N_i| x^{(d_{v_{i6}} + d_{v_{(i+1)0}})} = \\
 &= (3 \times 2^{n+1} - 6)x^5 + (5 \times 2^{n+2} - 19)x^4 + 2^{n+1}x^3, \\
 Z_{g2}(H, x) &= \sum_{uv \in E(G)} x^{d_u d_v} = \\
 &= |S_1| x^{(d_{v_{10}}d_{v_{01}})} + |S_2| x^{(d_{v_{01}}d_{v_{02}})} + \sum_{i=1}^n \sum_{t=1}^6 |M_{it}| x^{(d_{v_{i(t-1)}}d_{v_{it}})} + \\
 &+ \sum_{i=1}^n |N_i| x^{(d_{v_{i6}}d_{v_{(i+1)0}})} = \\
 &= (3 \times 2^{n+1} - 6)x^6 + (5 \times 2^{n+2} - 19)x^4 + 2^{n+1}x^2.
 \end{aligned}$$

Proof for Theorem 6

$$\begin{aligned}
 \bar{M}_1(H[n]) &= n(n-1)^2 - \sum_{i=1}^k |E_i|(d_{x_{j-1}} + d_{x_j}) = \\
 &= n(n-1)^2 - [|S_1|(d_{v_{10}} + d_{v_{01}}) + |S_2|(d_{v_{01}} + d_{v_{02}}) + \\
 &+ \sum_{i=1}^n \sum_{t=1}^6 |M_{it}|(d_{v_{i(t-1)}} + d_{v_{it}}) + \sum_{i=1}^n |N_i|(d_{v_{i6}} + d_{v_{(i+1)0}})] =
 \end{aligned}$$

$$\begin{aligned}
&= (28 \times 2^n - 24)(28 \times 2^n - 25)^2 - (29 \cdot 2^{n+2} - 106) = \\
&= 21952 \times 2^{3n} - 58016 \times 2^{2n} + 50984 \times 2^n - 14894, \\
\bar{M}_2(H[n]) &= n(n-1)^2 - \sum_{i=1}^k |E_i|(d_{x_{j-1}} d_{x_j}) = \\
&= n(n-1)^2 - [|S_1|(d_{v_{10}} d_{v_{01}}) + |S_2|(d_{v_{01}} d_{v_{02}}) + \\
&+ \sum_{i=1}^n \sum_{t=1}^6 |M_{it}|(d_{v_{i(t-1)}} d_{v_{it}}) + \sum_{i=1}^n |N_i|(d_{v_{i6}} d_{v_{(i+1)0}})] = \\
&= (28 \times 2^n - 24)(28 \times 2^n - 25)^2 - (15 \times 2^{n+3} - 112) = \\
&= 21952 \times 2^{3n} - 58016 \times 2^{2n} + 50980 \times 2^n - 14888,
\end{aligned}$$

where $n = 28 \times 2^n - 24$.

Proof for Theorem 7

$$\begin{aligned}
{}^v M_1(H[n]) &= |I|(d_{v_{01}})^{2v} + \sum_{i=1}^n \sum_{t=0}^6 |I_{it}|(d_{v_{it}})^{2v} + 2^{n+1}(d_{v_{(n+1)0}})^{2v} = \\
&= -2\{11 \times 2^{2v} + 3^{2v}\} + 2^{n+1}\{1 + 3^{2v} + 12 \times 2^{2v}\}, \\
{}^v M_2(H[n]) &= |S_1|(d_{v_{10}} d_{v_{01}})^v + |S_2|(d_{v_{01}} d_{v_{02}})^v + \\
&+ \sum_{i=1}^n \sum_{t=1}^6 |M_{it}|(d_{v_{i(t-1)}} d_{v_{it}})^v + \sum_{i=1}^n |N_i|(d_{v_{i6}} d_{v_{(i+1)0}})^v = \\
&= -6 \times 6^v - 19 \times 4^v + 2^{n+1}\{3 \times 6^v + 10 \times 4^v + 2^v\}.
\end{aligned}$$

Proof for Theorem 8

$$\begin{aligned}
HM(H[n]) &= |S_1|(d_{v_{10}} + d_{v_{01}})^2 + |S_2|(d_{v_{01}} + d_{v_{02}})^2 + \\
&+ \sum_{i=1}^n \sum_{t=1}^6 |M_{it}|(d_{v_{i(t-1)}} + d_{v_{it}})^2 + \sum_{i=1}^n |N_i|(d_{v_{i6}} + d_{v_{(i+1)0}})^2 = \\
&= 66 + 210 \sum_{i=1}^n 2^i + 50 \sum_{i=1}^{n-1} 2^i + 18 \cdot 2^n = \\
&= 463 \times 2^n - 404,
\end{aligned}$$

$$\begin{aligned}
 AZI(H[n]) &= |S_1| \left(\frac{d_{v_{10}} d_{v_{01}}}{d_{v_{10}} + d_{v_{01}} - 2} \right)^3 + |S_2| \left(\frac{d_{v_{01}} d_{v_{02}}}{d_{v_{01}} + d_{v_{02}} - 2} \right)^3 + \\
 &+ \sum_{i=1}^n \sum_{t=1}^6 |M_{it}| \left(\frac{d_{v_{i(t-1)}} d_{v_{it}}}{d_{v_{i(t-1)}} + d_{v_{it}}} \right)^3 + \sum_{i=1}^n |N_i| \left(\frac{d_{v_{i6}} d_{v_{(i+1)0}}}{d_{v_{i3}} + d_{v_{(i+1)0}} - 2} \right)^3 = \\
 &= 2(2)^3 + (2)^3 + \sum_{i=1}^n 2^{i+1} \{ (2)^3 + (2)^3 + (2)^3 + (2)^3 + (2)^3 + (2)^3 \} \\
 &+ \sum_{i=1}^{n-1} 2^{i+1} (2)^3 + 2^{n+1} (2)^3 = \\
 &= 7 \times 2^{n+5} - 200.
 \end{aligned}$$

Proof for Theorem 9

$$\begin{aligned}
 ABC_1(G[n]) &= |S_1| \sqrt{\frac{d_{v_{10}} + d_{v_{01}} - 2}{d_{v_{10}} d_{v_{01}}}} + |S_2| \sqrt{\frac{d_{v_{01}} + d_{v_{02}} - 2}{d_{v_{01}} d_{v_{02}}}} + \\
 &+ |S_3| \sqrt{\frac{d_{v_{02}} + d_{v_{03}} - 2}{d_{v_{02}} d_{v_{03}}}} + \sum_{i=1}^n 2^{i+1} \sum_{t=1}^3 \sqrt{\frac{d_{v_{i(t-1)}} + d_{v_{it}} - 2}{d_{v_{i(t-1)}} d_{v_{it}}}} + \\
 &+ \sum_{i=1}^{n-1} 2^{i+1} \sqrt{\frac{d_{v_{i3}} + d_{v_{(i+1)0}} - 2}{d_{v_{i3}} d_{v_{(i+1)0}}}} + 2^{n+1} \sqrt{\frac{d_{v_{n3}} + d_{v_{(n+1)0}} - 2}{d_{v_{n3}} d_{v_{(n+1)0}}}} = \\
 &= \frac{5}{\sqrt{2}} + \sum_{i=1}^n 2^{i+1} \left(\frac{3}{\sqrt{2}} \right) + \sum_{i=1}^{n-1} 2^{i+1} \left(\frac{1}{\sqrt{2}} \right) + 2^{n+1} \left(\frac{1}{\sqrt{2}} \right) = \\
 &= \frac{-11}{\sqrt{2}} + 2^n \times \frac{16}{\sqrt{2}}.
 \end{aligned}$$

Proof for Theorem 10

If uv is an edge in G then m_u is the number of vertices closer to u than to v . As $v_{01}v_{02} \in E(G)$, the number of vertices closer to v_{01} than to v_{02} are:

$$\begin{aligned}
 m_{v_{01}} &= 2 + 4(2) + 4(2^2) + \dots + 4(2^n) = 2 + 4(2 + 2^2 + \dots + 2^n) = \\
 &= 2 + 8(2^n - 1) = 8 \times 2^n - 6.
 \end{aligned}$$

Similarly, $m_{v_{02}} = 8 \times 2^n - 5$ and $m_{v_{it}} = 8 \times 2^{n-i+\delta_{0t}} - (3 + t + 4\delta_{0t})$, where $1 \leq i \leq n$ and $0 \leq t \leq 3$, and $m_{v_{(i+1)0}} = 8 \times 2^{n-i} - 7$. Now, by using Automorphism group action on the vertices and edges of $G[n]$ and Lemma 2, one obtains:

$$\begin{aligned}
ABC_2(G[n]) &= |S_1| \sqrt{\frac{m_{v_{10}} + m_{v_{01}} - 2}{m_{v_{10}} m_{v_{01}}}} + |S_2| \sqrt{\frac{m_{v_{01}} + m_{v_{02}} - 2}{m_{v_{01}} m_{v_{02}}}} + \\
&+ |S_3| \sqrt{\frac{m_{v_{02}} + m_{v_{03}} - 2}{m_{v_{02}} m_{v_{03}}}} + \sum_{i=1}^n 2^{i+1} \sum_{t=1}^3 \sqrt{\frac{m_{v_{i(t-1)}} + m_{v_{it}} - 2}{m_{v_{i(t-1)}} m_{v_{it}}}} + \\
&+ \sum_{i=1}^{n-1} 2^{i+1} \sqrt{\frac{m_{v_{i3}} + m_{v_{(i+1)0}} - 2}{m_{v_{i3}} m_{v_{(i+1)0}}}} + 2^{n+1} \sqrt{\frac{m_{v_{n3}} + m_{v_{(n+1)0}} - 2}{m_{v_{n3}} m_{v_{(n+1)0}}}} = \\
&= \alpha_1 \left[\frac{2}{\sqrt{\beta_1}} + \frac{2}{\sqrt{\beta_1 + 3}} + \frac{1}{\sqrt{\beta_1 + 4}} + \sum_{i=1}^n \left\{ \frac{1}{\sqrt{\gamma_1 - 16(2^{n-i}) - 64(2^n) + 3}} \right. \right. \\
&\quad + \frac{1}{\sqrt{\gamma_1 - 80(2^n) + 4}} + \frac{1}{\sqrt{\gamma_1 + 16(2^{n-i}) - 96(2^n) + 3}} + \\
&\quad \left. \left. + \frac{1}{\sqrt{\gamma_1 + 32(2^{n-i}) - 112(2^n)}} \right\} \right].
\end{aligned}$$

Proof for Theorem 11

As $S_{v_{01}} = 2 + 3 + 2 = 7$, similarly, $S_{v_{02}} = 6$, $S_{v_{10}} = 9$, $S_{v_{11}} = 7$, $S_{v_{12}} = 6$, $1 \leq i \leq n$, $S_{v_{i3}} = 7$, $1 \leq i \leq n-1$, $S_{v_{ns}} = 5$ and $S_{v_{(n+1)0}} = 3$, $S_{v_{it}} = 6 + 3\delta_{0t} + \delta_{1t} + \delta_{3t}$ where $1 \leq i \leq n-1$ and $0 \leq t \leq 3$.

$$= \left\{ \sqrt{\frac{5}{18}} - 6\sqrt{\frac{11}{42}} - 6\sqrt{\frac{14}{63}} \right\} + 2^n \left\{ 6\sqrt{\frac{14}{63}} + 6\sqrt{\frac{11}{42}} + 2\sqrt{\frac{9}{30}} + 2\sqrt{\frac{3}{4}} \right\}$$

Proof:

As $\epsilon_{v_{02}} = \tau_1 = \epsilon_{v_{04}}$, $\epsilon_{v_{01}} = \tau_1 + 1 = \epsilon_{v_{03}}$, $\epsilon_{v_{(n+1)0}} = \tau_1 + 6$ and $\epsilon_{v_{it}} = \tau_1 + 4i + t - 2$, where $1 \leq i \leq n$ and $0 \leq t \leq 3$. Here τ_1 is defined² as $\tau_1 = 4n + 3$.

Proof for Theorem 12

$$\begin{aligned}
ABC_5(G[n]) &= |S_1| \sqrt{\frac{\epsilon_{v_{10}} + \epsilon_{v_{01}} - 2}{\epsilon_{v_{10}} \epsilon_{v_{01}}}} + |S_2| \sqrt{\frac{\epsilon_{v_{01}} + \epsilon_{v_{02}} - 2}{\epsilon_{v_{01}} \epsilon_{v_{02}}}} + \\
&+ |S_3| \sqrt{\frac{\epsilon_{v_{02}} + \epsilon_{v_{03}} - 2}{\epsilon_{v_{02}} \epsilon_{v_{03}}}} + \sum_{i=1}^n 2^{i+1} \sum_{t=1}^3 \sqrt{\frac{\epsilon_{v_{i(t-1)}} + \epsilon_{v_{it}} - 2}{\epsilon_{v_{i(t-1)}} \epsilon_{v_{it}}}} + \\
&+ \sum_{i=1}^{n-1} 2^{i+1} \sqrt{\frac{\epsilon_{v_{i3}} + \epsilon_{v_{(i+1)0}} - 2}{\epsilon_{v_{i3}} \epsilon_{v_{(i+1)0}}}} + 2^{n+1} \sqrt{\frac{\epsilon_{v_{n3}} + \epsilon_{v_{(n+1)0}} - 2}{\epsilon_{v_{n3}} \epsilon_{v_{(n+1)0}}}} =
\end{aligned}$$

$$\begin{aligned}
 &= 2\sqrt{\frac{2\tau_1+1}{(\tau_1+2)(\tau_1+1)}} + 2\sqrt{\frac{2\tau_1-1}{\tau_1(\tau_1+1)}} + \frac{\sqrt{2\tau_1-2}}{\tau_1} + \\
 &+ \sum_{i=1}^n 2^{i+1} \left\{ \sqrt{\frac{2\tau_1+8i+1}{(\tau_1+4i+1)(\tau_1+4i+2)}} + \sum_{t=1}^3 \sqrt{\frac{2\tau_1+8i+2t-8}{(\tau_1+4i+t-2)(\tau_1+4i+t-3)}} \right\} = \\
 &= 2\sqrt{\frac{8n+7}{(4n+5)(4n+4)}} + 2\sqrt{\frac{8n+5}{(4n+3)(4n+4)}} + \frac{\sqrt{8n+4}}{4n+3} + \\
 &+ \sum_{i=1}^n 2^{i+1} \left\{ \sqrt{\frac{8n+8i+7}{(4n+4i+4)(4n+4i+5)}} + \sum_{t=1}^3 \sqrt{\frac{8n+8i+2t-2}{(4n+4i+t+1)(4n+4i+t)}} \right\}.
 \end{aligned}$$

Proof for Theorem 13

$$\begin{aligned}
 ABC_1(H[n]) &= |S_1| \sqrt{\frac{d_{v_{10}} + d_{v_{01}} - 2}{d_{v_{10}} d_{v_{01}}}} + |S_2| \sqrt{\frac{d_{v_{01}} + d_{v_{02}} - 2}{d_{v_{01}} d_{v_{02}}}} + \\
 &+ \sum_{i=1}^n 2^{i+1} \sum_{t=1}^6 \sqrt{\frac{d_{v_{i(t-1)}} + d_{v_{it}} - 2}{d_{v_{i(t-1)}} d_{v_{it}}}} + \sum_{i=1}^{n-1} 2^{i+1} \sqrt{\frac{d_{v_{i6}} + d_{v_{(i+1)0}} - 2}{d_{v_{i6}} d_{v_{(i+1)0}}}} + \\
 &+ 2^{n+1} \sqrt{\frac{d_{v_{n6}} + d_{v_{(n+1)0}} - 2}{d_{v_{n6}} d_{v_{(n+1)0}}}} = \\
 &= \frac{3}{\sqrt{2}} + \sum_{i=1}^n 2^{i+1} \left(\frac{6}{\sqrt{2}}\right) + \sum_{i=1}^{n-1} 2^{i+1} \left(\frac{1}{\sqrt{2}}\right) + 2^{n+1} \left(\frac{1}{\sqrt{2}}\right) = \\
 &= \frac{-25}{\sqrt{2}} + 2^n \times \frac{28}{\sqrt{2}}
 \end{aligned}$$

Proof for Theorem 14

It is noted that $m_{v_{01}} = 14 \times 2^n - 12, m_{v_{02}} = 14 \times 2^n - 11$ and $m_{v_{it}} = 14 \times 2^{n-i} \delta_{0t} - (6+t+7\delta_{0t})$ where $1 \leq i \leq n$ and $0 \leq t \leq 6$ and $m_{v_{(i+1)0}} = 14 \times 2^{n-i} - 10$. Now by using Automorphism group action on the vertices and edges of $H[n]$ and Lemma 2, one obtains:

$$\begin{aligned}
 ABC_2(H[n]) &= |S_1| \sqrt{\frac{m_{v_{10}} + m_{v_{01}} - 2}{m_{v_{10}} m_{v_{01}}}} + |S_2| \sqrt{\frac{m_{v_{01}} + m_{v_{02}} - 2}{m_{v_{01}} m_{v_{02}}}} + \\
 &+ \sum_{i=1}^n 2^{i+1} \sum_{t=1}^6 \sqrt{\frac{m_{v_{i(t-1)}} + m_{v_{it}} - 2}{m_{v_{i(t-1)}} m_{v_{it}}}} + \sum_{i=1}^{n-1} 2^{i+1} \sqrt{\frac{m_{v_{i3}} + m_{v_{(i+1)0}} - 2}{m_{v_{i3}} m_{v_{(i+1)0}}}} +
 \end{aligned}$$

$$\begin{aligned}
& +2^{n+1} \sqrt{\frac{m_{v_{n6}} + m_{v_{(n+1)0}} - 2}{m_{v_{n6}} m_{v_{(n+1)0}}} = \\
& = \alpha_2 \left[\frac{2}{\sqrt{\beta_2}} + \frac{1}{\sqrt{\beta_2 + 1}} + \sum_{i=1}^n \left\{ \frac{1}{\sqrt{\gamma_2 - 140(2^{n-i}) - 196(2^n)}} + \right. \right. \\
& + \frac{1}{\sqrt{\gamma_2 - 112(2^{n-i}) - 224(2^n) + 9}} + \frac{1}{\sqrt{\gamma_2 - 84(2^{n-i}) - 252(2^n) + 16}} + \\
& + \frac{2}{\sqrt{\gamma_2 - 56(2^{n-i}) - 280(2^n) + 21}} + \frac{1}{\sqrt{\gamma_2 - 28(2^{n-i}) - 308(2^n) + 24}} + \\
& \left. \left. + \frac{1}{\sqrt{\gamma_2 - 336(2^n) + 25}} \right\} \right].
\end{aligned}$$

Proof for Theorem 15

$S_{v_{01}} = 7$, $S_{v_{i0}} = 9$, $S_{v_{n1}} = 7$, $S_{v_{i2}} = S_{v_{i3}} = S_{v_{i4}} = S_{v_{i5}} = 6$, $1 \leq i \leq n$, $S_{v_{i6}} = 7$,
 $1 \leq i \leq n-1$, $S_{v_{n6}} = 5$ and $S_{v_{(n+1)0}} = 3$. $S_{v_{it}} = 6 + \delta_{1t} + \delta_{2t} + \delta_{3t}$,

where $1 \leq i \leq n-1$ and $0 \leq t \leq 6$.

$$\begin{aligned}
ABC_4(H[n]) &= |S_1| \sqrt{\frac{S_{v_{i0}} + S_{v_{01}} - 2}{S_{v_{i0}} S_{v_{01}}}} + |S_2| \sqrt{\frac{S_{v_{02}} + S_{v_{01}} - 2}{S_{v_{02}} S_{v_{01}}}} + \\
& + \sum_{i=1}^n 2^{i+1} \sum_{t=1}^6 \sqrt{\frac{S_{v_{i(t-1)}} + S_{v_{it}} - 2}{S_{v_{i(t-1)}} S_{v_{it}}}} + \sum_{i=1}^{n-1} 2^{i+1} \sqrt{\frac{S_{v_{i(6)}} + S_{v_{(i+1)0}} - 2}{S_{v_{i(6)}} S_{v_{(i+1)0}}}} + \\
& + 2^{n+1} \sqrt{\frac{S_{v_{n(6)}} + S_{v_{(n+1)0}} - 2}{S_{v_{n(6)}} S_{v_{(n+1)0}}}} = \\
& = \left\{ -2\sqrt{\frac{14}{63}} + 12\sqrt{\frac{12}{49}} - 8\sqrt{\frac{11}{42}} - 12\sqrt{\frac{5}{18}} \right\} + \\
& + 2^n \left\{ 8\sqrt{\frac{14}{63}} + 6\sqrt{\frac{11}{42}} + 12\sqrt{\frac{5}{18}} + 2\sqrt{\frac{2}{5}} \right\}
\end{aligned}$$

Proof for Theorem 16

As $\epsilon_{v_{01}} = \tau_2 = \epsilon_{v_{02}}$, $\epsilon_{v_{(n+1)0}} = \tau_2 + 7n + 1$ and $\epsilon_{v_{it}} = \tau_2 + 7i + t - 6$, where $1 \leq i \leq n$ and $0 \leq t \leq 6$. Here, $\tau_2 = 7n + 2$.

$$\begin{aligned}
 ABC_5(H[n]) &= |S_1| \sqrt{\frac{\epsilon_{v_{10}} + \epsilon_{v_{01}} - 2}{\epsilon_{v_{10}} \epsilon_{v_{01}}}} + |S_2| \sqrt{\frac{\epsilon_{v_{01}} + \epsilon_{v_{02}} - 2}{\epsilon_{v_{01}} \epsilon_{v_{02}}}} + \\
 &+ \sum_{i=1}^n 2^{i+1} \sum_{t=1}^6 \sqrt{\frac{\epsilon_{v_{i(t-1)}} + \epsilon_{v_{it}} - 2}{\epsilon_{v_{i(t-1)}} \epsilon_{v_{it}}}} + \sum_{i=1}^{n-1} 2^{i+1} \sqrt{\frac{\epsilon_{v_{i3}} + \epsilon_{v_{(i+1)0}} - 2}{\epsilon_{v_{i3}} \epsilon_{v_{(i+1)0}}}} + \\
 &\quad + 2^{n+1} \sqrt{\frac{\epsilon_{v_{n6}} + \epsilon_{v_{(n+1)0}} - 2}{\epsilon_{v_{n6}} \epsilon_{v_{(n+1)0}}}} \\
 &= 2 \sqrt{\frac{2\tau_2 - 1}{\tau_2(\tau_2 + 1)}} + \frac{\sqrt{2\tau_2 - 2}}{\tau_2} + \sum_{i=1}^n 2^{i+1} \left\{ \sqrt{\frac{2\tau_2 + 14i - 11}{(\tau_2 + 7i)(\tau_2 + 7i + 1)}} \right. \\
 &\quad \left. + \sum_{t=1}^6 \sqrt{\frac{2\tau_2 + 14i + 2t - 15}{(\tau_2 + 7i + t - 7)(\tau_2 + 7i + t - 6)}} \right\} \\
 &= 2 \sqrt{\frac{14n + 3}{(7n + 2)(7n + 3)}} + \frac{\sqrt{14n + 2}}{7n + 2} + \sum_{i=1}^n 2^{i+1} \left\{ \sqrt{\frac{14n + 14i + 3}{(7n + 7i + 2)(7n + 7i + 3)}} \right. \\
 &\quad \left. + \sum_{t=1}^6 \sqrt{\frac{14n + 14i + 2t - 11}{(7n + 7i + t - 5)(7n + 7i + t - 4)}} \right\}
 \end{aligned}$$

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