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On the Generalized *ABC* Index of Graphs

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Abstract

The atom-bond connectivity and the generalized atom-bond connectivity indices have shown to be useful in the QSPR/QSAR researches. In particular, the atom-bond connectivity index has been applied to study the stability of alkanes and the strain energy of cycloalkanes. In this paper we obtain some bounds on these indices in terms of graph parameters. To obtain these bounds we use the mathematical tools from analysis. Some of these bounds for ABC_α improve, when $\alpha = 1/2$, known results on the ABC index.

1 Introduction

A single number, representing a chemical structure in graph-theoretical terms via the molecular graph, is called a topological index if it correlates with a molecular property.

Topological indices are used to understand physicochemical properties of chemical compounds. Topological indices are interesting since they capture some of the properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener.

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Topological indices based on end-vertex degrees of edges have been used over almost 50 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best known such descriptors are the Randić connectivity index (R) and the Zagreb indices.

The *atom-bond connectivity index* (ABC-index) is a useful topological index employed in studying the stability of alkanes and the strain energy of cycloalkanes. The atom-bond connectivity index of a graph G was defined in [8] as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \,,$$

where uv denotes the edge of the graph G connecting the vertices u and v, and d_u is the degree of the vertex u.

The *generalized atom-bond connectivity index* was defined in [9] as

$$ABC_\alpha(G) = \sum_{uv \in E(G)} \Big(\frac{d_u + d_v - 2}{d_u d_v}\Big)^\alpha .$$

for any $\alpha \in \mathbb{R} \setminus \{0\}$. Note that $ABC_{1/2}$ is the ABC-index and ABC_{-3} is the augmented Zagreb index.

There are a lot of papers studying the ABC and ABC_α indices (see, e.g., [2, 3, 5, 6, 9, 10, 12–17]). Recently, Estrada [7] referred to the above generalization ABC_α as the generalized ABC index, and provided a probabilistic interpretation that fits very well with the chemical intuition for understanding the capacity of ABC-like indices to describe the energetics of alkanes. Chen at el. [3] characterized the graphs having the maximal ABC_α value for $\alpha < 0$ among all connected graphs with given order and vertex connectivity, edge connectivity, or matching number. Very recently, we presented some optimization results for ABC_α of the connected graph G [6]. In [16], Tan et al. determine the maximum value of ABC_α together with the corresponding extremal graphs in the class of graphs with n vertices and maximum degree Δ for $0 < \alpha \leq \frac{1}{2}$. In this paper we obtain new inequalities for these indices. Some of these inequalities for ABC_α improve, when $\alpha = 1/2$, known results on the ABC index.

Throughout this work, $G = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) graph without isolated vertices. We denote by Δ, δ, n, m the maximum degree, the minimum degree and the cardinality of the set of vertices and edges of G, respectively.

2 Inequalities involving ABC_α

Recall that an *isolated edge* in a graph G is a connected component of G isomorphic to a path graph P_2.

Theorem 1. *Let G be a graph with m edges, maximum degree Δ and minimum degree δ, and $\alpha > 0$. Denote by m_2 the cardinality of the set of isolated edges in G.*

(1) *If $\delta > 1$, then*

$$\Big(\frac{2\Delta-2}{\Delta^2}\Big)^\alpha m \le ABC_\alpha(G) \le \Big(\frac{2\delta-2}{\delta^2}\Big)^\alpha m.$$

The equality in each bound is attained if G is a regular graph. If $\Delta > 2$, then the equality in the lower bound is attained if and only if G is a regular graph. If $\delta > 2$, then the equality in the upper bound is attained if and only if G is a regular graph.

(2) *If $\delta = 1$, then*

$$\Big(\frac{2\Delta-2}{\Delta^2}\Big)^\alpha (m-m_2) \le ABC_\alpha(G) \le \Big(\frac{\Delta-1}{\Delta}\Big)^\alpha (m-m_2).$$

The equality in the lower bound is attained if G is a union of a regular graph and m_2 isolated edges; if $\Delta > 2$, then the equality in this bound is attained if and only if G is a union of a regular graph and m_2 isolated edges. The equality in the upper bound is attained if and only if G is a union of star graphs $S_{\Delta+1}$ and m_2 isolated edges.

Proof. It is well-known that

$$f(x,y) = \frac{x+y-2}{xy}$$

is a decreasing function in each variable on $[2,\infty)\times[2,\infty)$ and strictly decreasing on $(2,\infty)\times(2,\infty)$. Hence,

$$\frac{2\Delta-2}{\Delta^2} \le f(x,y) \le \frac{2\delta-2}{\delta^2} \qquad (1)$$

for every $x, y \in [\delta,\Delta]$.

First we assume that $\delta > 1$. Therefore,

$$\frac{2\Delta-2}{\Delta^2} \le \frac{d_u+d_v-2}{d_u d_v} \le \frac{2\delta-2}{\delta^2}$$

for every $uv \in E(G)$. Furthermore, if $\Delta > 2$, then the left hand inequality is strict if and only if $(d_u, d_v) \ne (\Delta,\Delta)$; if $\delta > 2$, then the right hand inequality is strict if and only if $(d_u, d_v) \ne (\delta,\delta)$. Hence,

$$\Big(\frac{2\Delta-2}{\Delta^2}\Big)^\alpha m \le ABC_\alpha(G) \le \Big(\frac{2\delta-2}{\delta^2}\Big)^\alpha m.$$

If $\Delta > 2$, then the equality in the lower bound is attained if and only if G is a regular graph. If $\delta > 2$, then the equality in the upper bound is attained if and only if G is a regular graph.

Also, if G is a regular graph, then the lower and upper bounds are the same, and they are equal to $ABC_\alpha(G)$.

Next we assume that $\delta = 1$. Since $ABC_\alpha(P_2) = 0$, it suffices to prove the statement when G does not have isolated edges, i.e., $m_2 = 0$. Thus, $\max\{d_u, d_v\} \geq 2$ for every $uv \in E(G)$. Since $f(1, y) \leq (y-1)/y$ is strictly increasing on $[2, \infty)$, we have

$$\frac{1}{2} \leq f(1, y) \leq \frac{\Delta - 1}{\Delta}$$

for every $y \in [2, \Delta]$. If $x, y \in [2, \Delta]$, then (1) gives

$$\frac{2\Delta - 2}{\Delta^2} \leq f(x, y) \leq \frac{1}{2}\,.$$

Hence,

$$\frac{2\Delta - 2}{\Delta^2} \leq \frac{d_u + d_v - 2}{d_u d_v} \leq \frac{\Delta - 1}{\Delta}$$

for every $uv \in E(G)$. Furthermore, if $\Delta > 2$, then the left hand inequality is strict if and only if $(d_u, d_v) \neq (\Delta, \Delta)$; the right hand inequality is strict if and only if $\{d_u, d_v\} \neq \{1, \Delta\}$.

Hence,

$$\Big(\frac{2\Delta - 2}{\Delta^2}\Big)^\alpha m \leq ABC_\alpha(G) \leq \Big(\frac{\Delta - 1}{\Delta}\Big)^\alpha m.$$

The equality in the lower bound is attained if G is a regular graph. If $\Delta > 2$, then the equality in the lower bound is attained if and only if G is a regular graph. The equality in the upper bound is attained if and only if every edge in $E(G)$ has a vertex of degree 1 and the other vertex with degree Δ, i.e., G is a union of star graphs $S_{\Delta+1}$. ■

Recall that $ABC_\alpha(G)$ is not well-defined if $\alpha < 0$ and G has an isolated edge. The argument in the proof of Theorem 1 gives directly the following result for $\alpha < 0$.

Theorem 2. *Let G be a graph without isolated edges, with m edges, maximum degree Δ, minimum degree δ, and $\alpha < 0$.*

(1) *If $\delta > 1$, then*

$$\Big(\frac{2\delta - 2}{\delta^2}\Big)^\alpha m \leq ABC_\alpha(G) \leq \Big(\frac{2\Delta - 2}{\Delta^2}\Big)^\alpha m.$$

The equality in each bound is attained if G *is a regular graph. If* $\delta > 2$*, then the equality in the lower bound is attained if and only if* G *is a regular graph. If* $\Delta > 2$*, then the equality in the upper bound is attained if and only if* G *is a regular graph.*

(2) *If* $\delta = 1$ *and* $\Delta > 1$*, then*

$$\Big(\frac{\Delta - 1}{\Delta} \Big)^{\alpha} m \le ABC_{\alpha}(G) \le \Big(\frac{2\Delta - 2}{\Delta^2} \Big)^{\alpha} m.$$

The equality in the lower bound is attained if and only if G *is a union of star graphs* $S_{\Delta+1}$*. The equality in the upper bound is attained if* G *is a regular graph; if* $\Delta > 2$*, then the equality in this bound is attained if and only if* G *is a regular graph.*

Note that if $2m/\Delta$ is an integer, with $m, \Delta \in \mathbb{Z}$ and $2 \le \Delta < m$, then there exists a (connected) Δ-regular graph with m edges (see [1, Lemma 2.6]). Also, if m/Δ is an integer, then there exists a union of star graphs $S_{\Delta+1}$ with m edges. Hence, in many cases Theorems 1 and 2 solve extremal problems, since they provide the extremal graphs for ABC_{α} with fixed number of edges and maximum or minimum degree.

Corollary 1. *Let* G *be a graph with* m *edges, maximum degree* Δ *and minimum degree* δ*. Let* m_2 *be the cardinality of the set of isolated edges in* G*.*

(1) *If* $\delta > 1$*, then*

$$\frac{\sqrt{2\Delta - 2}}{\Delta}\, m \le ABC(G) \le \frac{\sqrt{2\delta - 2}}{\delta}\, m.$$

(2) *If* $\delta = 1$*, then*

$$\frac{\sqrt{2\Delta - 2}}{\Delta}\, (m - m_2) \le ABC(G) \le \sqrt{\frac{\Delta - 1}{\Delta}}\, (m - m_2).$$

Remark 2. (1) In [4, Theorem 6] appears the inequality

$$ABC(G) \le \frac{\Delta + \delta}{\sqrt{\Delta\delta}}\, m.$$

Note this inequality is improved by the upper bound in Corollary 1 for every Δ and δ.

(2) In [4, Theorem 6] appears the inequality

$$ABC(G) \ge \frac{\sqrt{2\delta - 2}}{\Delta}\, m,$$

correcting a typo in [11, Theorem 3.1]. Note that this inequality is improved by the lower bound in Corollary 1 for every $\Delta > \delta$.

Recall that a *chemical graph* is a connected graph with maximum degree at most 4. Next, we improve some inequalities in Theorems 1 and 2 for chemical graphs. First of all, we need some technical results.

Lemma 3. *Let $a_1, a_2, \dots, a_n > 0$ and $c_1, c_2, \dots, c_n \in \mathbb{R} \setminus \{0\}$. The function*

$$F(x) = c_1 a_1^x + c_2 a_2^x + \cdots + c_n a_n^x$$

has at most $n-1$ real zeros taking into account their multiplicities.

Proof. Without loss of generality we can assume that $a_i \neq a_j$ for every $i \neq j$. Let us prove it by induction on n. The result is true for $n = 1$. Assume that the result holds for $n-1$ and let us prove it for n. By dividing by a_1^x, it suffices to show that the function

$$f(x) = c_1 + c_2 A_2^x + \cdots + c_n A_n^x,$$

with $A_2, \dots, A_n \in \mathbb{R}^+ \setminus \{1\}$ (since $a_i \neq a_j$ for every $i \neq j$), has at most $n-1$ real zeros taking into account their multiplicities.

Let $x_1, \dots, x_k$ be the real zeros of f, where $x_1, \dots, x_r$ $(0 \le r \le k)$ have multiplicities $n_1, \dots, n_r > 1$, respectively, and $x_{r+1}, \dots, x_k$ have multiplicity 1. Thus, f has exactly $k - r + n_1 + \cdots + n_r$ real zeros taking into account their multiplicities.

Thus, $x_1, \dots, x_r$ are real zeros of f' with multiplicities $n_1 - 1, \dots, n_r - 1$, respectively. Also, Rolle's theorem gives that f' has at least $k-1$ additional real zeros.

Since

$$f'(x) = c_2 A_2^x \log A_2 + \cdots + c_n A_n^x \log A_n,$$

and $c_j \log A_j \neq 0$, the induction hypothesis gives that f' has at most $n-2$ real zeros taking into account their multiplicities. Hence,

$$k - 1 + n_1 - 1 + \cdots + n_r - 1 = k - 1 - r + n_1 + \cdots + n_r \le n - 2,$$

and f has exactly $k - r + n_1 + \cdots + n_r \le n-1$ real zeros taking into account their multiplicities. ■

Lemma 4. *Let $0 < a_1 < a_2 \le a_3 < a_4$, $c_1, c_2, c_3, c_4 > 0$ with $c_1 + c_4 = c_2 + c_3$, and the function*

$$H(x) = c_1 a_1^x + c_4 a_4^x - c_2 a_2^x - c_3 a_3^x.$$

(1) *If* $c_1 \log a_1 + c_4 \log a_4 > c_2 \log a_2 + c_3 \log a_3$, *then there exists a unique negative zero* x_0 *of* H, *and* $H(x) > 0$ *if and only if* $x \in (-\infty, x_0) \cup (0, \infty)$.

(2) *If* $c_1 \log a_1 + c_4 \log a_4 < c_2 \log a_2 + c_3 \log a_3$, *then there exists a unique positive zero* x_0 *of* H, *and* $H(x) > 0$ *if and only if* $x \in (-\infty, 0) \cup (x_0, \infty)$.

Proof. Since

$$H'(x) = c_1 a_1^x \log a_1 + c_4 a_4^x \log a_4 - c_2 a_2^x \log a_2 - c_3 a_3^x \log a_3,$$

if $c_1 \log a_1 + c_4 \log a_4 > c_2 \log a_2 + c_3 \log a_3$, then $H'(0) > 0$. Since $H(0) = 0$ by $c_1 + c_4 = c_2 + c_3$, there exists $\varepsilon > 0$ with $H < 0$ on $(-\varepsilon, 0)$. Since $0 < a_1 < a_2 \leq a_3 < a_4$, we have $H(x) > 0$ when $|x| >> 1$. Lemma 3 gives that H has at most 3 real zeros taking into account their multiplicities. Since H changes it sign at 0 and at a negative point, and $H(x) > 0$ when $|x| >> 1$, it has at most 2 different real zeros. Thus, there exists a unique negative zero x_0 of H, and $H(x) > 0$ if and only if $x \in (-\infty, x_0) \cup (0, \infty)$.

If $c_1 \log a_1 + c_4 \log a_4 < c_2 \log a_2 + c_3 \log a_3$, then a similar argument gives the result. ■

Lemma 4 has the following consequence.

Corollary 5. *Let* $0 < a_1 < a_2 < a_3$, $c_1, c_3 > 0$ *and the function*

$$H(x) = c_1 a_1^x + c_3 a_3^x - (c_1 + c_3) a_2^x.$$

(1) *If* $c_1 \log a_1 + c_3 \log a_3 > (c_1 + c_3) \log a_2$, *then there exists a unique negative zero* x_0 *of* H, *and* $H(x) > 0$ *if and only if* $x \in (-\infty, x_0) \cup (0, \infty)$.

(2) *If* $c_1 \log a_1 + c_3 \log a_3 < (c_1 + c_3) \log a_2$, *then there exists a unique positive zero* x_0 *of* H, *and* $H(x) > 0$ *if and only if* $x \in (-\infty, 0) \cup (x_0, \infty)$.

The argument in the proof of Lemma 4 also gives the following result.

Lemma 6. *Let* $0 < a_1 < a_2 < a_3$, $0 < a_1 < b < a_3$, $c_1, c_2, c_3 > 0$ *and the function*

$$H(x) = c_1 a_1^x + c_2 a_2^x + c_3 a_3^x - (c_1 + c_2 + c_3) b^x.$$

(1) *If* $c_1 \log a_1 + c_2 \log a_2 + c_3 \log a_3 > (c_1 + c_2 + c_3) \log b$, *then there exists a unique negative zero* x_0 *of* H, *and* $H(x) > 0$ *if and only if* $x \in (-\infty, x_0) \cup (0, \infty)$.

(2) *If* $c_1 \log a_1 + c_2 \log a_2 + c_3 \log a_3 < (c_1 + c_2 + c_3) \log b$, *then there exists a unique positive zero* x_0 *of* H, *and* $H(x) > 0$ *if and only if* $x \in (-\infty, 0) \cup (x_0, \infty)$.

Lemma 7. *Let $0 < a_1 < a_2 < a_3$, $0 < b_1 < b_2$, $c_1, c_2, c_3, k_1, k_2 > 0$, with $c_1 + c_2 + c_3 = k_1 + k_2$, $b_1 < a_1$ and $b_2 < a_3$, and the function*

$$H(x) = c_1 a_1^x + c_2 a_2^x + c_3 a_3^x - k_1 b_1^x - k_2 b_2^x.$$

If $c_1 \log a_1 + c_2 \log a_2 + c_3 \log a_3 < k_1 \log b_1 + k_2 \log b_2$, then there exist a unique negative zero x_1 of H and a unique positive zero x_2 of H, and $H(x) > 0$ if and only if $x \in (x_1, 0) \cup (x_2, \infty)$.

Proof. Since

$$H'(x) = c_1 a_1^x \log a_1 + c_2 a_2^x \log a_2 + c_3 a_3^x \log a_3 - k_1 b_1^x \log b_1 - k_2 b_2^x \log b_2,$$

and $c_1 \log a_1 + c_2 \log a_2 + c_3 \log a_3 < k_1 \log b_1 + k_2 \log b_2$, we have $H'(0) < 0$. Since $c_1 + c_2 + c_3 = k_1 + k_2$ gives $H(0) = 0$, there exists $\varepsilon > 0$ with $H > 0$ on $(-\varepsilon, 0)$ and $H < 0$ on $(0, \varepsilon)$. Since $b_1 < a_1$ and $b_2 < a_3$, we have $H(x) < 0$ when $x << -1$ and $H(x) > 0$ when $x >> 1$. Hence, H has a negative zero and a positive zero. Lemma 3 gives that H has at most 4 real zeros taking into account their multiplicities. Hence, H has exactly 3 different real zeros $x_1 < 0 < x_2$. ■

Given integer numbers a, b, k, we write $a \equiv b \,(\text{mod}\, k)$ if $a - b$ is an integer multiple of k. In this case, a and b are said to be *congruent modulo k*.

If $m \geq 6$ is an integer with $m \equiv 1 \,(\text{mod}\, 3)$, then we denote by $\mathcal{A}_m$ the set of graphs with m edges such that a vertex has degree 2 and the other vertices have degree 3. Since $m-1$ is an integer multiple of 3 (grater than 3), there exists a 3-regular graph with $m-1$ edges (see, e.g., [1]); if we replace any fixed edge of this graph by a path P_3, then we obtain a graph in $\mathcal{A}_m$ (and so, $\mathcal{A}_m \neq \emptyset$). Obviously, any graph in $\mathcal{A}_m$ can be obtained in this way from a 3-regular graph with $m-1$ edges.

If $m \geq 6$ is an integer with $m \equiv 2 \,(\text{mod}\, 3)$, then we denote by $\mathcal{B}_m$ the set of graphs with m edges such that two adjacent vertices have degree 2 and the other vertices have degree 3. Since $m-2$ is an integer multiple of 3 (grater than 3), there exists a 3-regular graph with $m-2$ edges (see, e.g., [1]); if we replace any fixed edge of this graph by a path P_4, then we obtain a graph in $\mathcal{B}_m$. Any graph in $\mathcal{B}_m$ can be obtained in this way from a 3-regular graph with $m-2$ edges.

If $m \geq 6$ is an integer with $m \equiv 2 \,(\text{mod}\, 3)$, then we denote by $\mathcal{C}_m$ the set of graphs with m edges such that a vertex has degree 1 and the other vertices have degree 3. Since

$m-1 \equiv 1 \pmod 3$, there exists a graph in $\mathcal{A}_{m-1}$; if we add a pendant edge to its single vertex with degree 2, then we obtain a graph in $\mathcal{C}_m$. Any graph in $\mathcal{C}_m$ can be obtained in this way from a graph in $\mathcal{A}_{m-1}$.

Theorem 3. *Let G be a connected graph with $m \geq 6$ edges and maximum degree 3, and $\alpha \in \mathbb{R}$.*

(1) *Assume that $m \equiv 0 \pmod 3$. Then*

$$m\,\frac{4^\alpha}{9^\alpha} \leq ABC_\alpha(G), \qquad \text{if } \alpha > 0,$$
$$m\,\frac{4^\alpha}{9^\alpha} \geq ABC_\alpha(G), \qquad \text{if } \alpha < 0.$$

The equality in each bound is attained if and only if G is a 3-regular graph.

(2) *Assume that $m \equiv 1 \pmod 3$. Then*

$$(m-2)\,\frac{4^\alpha}{9^\alpha} + 2\,\frac{1}{2^\alpha} \leq ABC_\alpha(G), \qquad \text{if } \alpha > 0,$$
$$(m-2)\,\frac{4^\alpha}{9^\alpha} + 2\,\frac{1}{2^\alpha} \geq ABC_\alpha(G), \qquad \text{if } \alpha < 0.$$

The equality in each bound is attained if and only if G is a graph in $\mathcal{A}_m$.

(3) *Assume that $m \equiv 2 \pmod 3$. Then*

$$(m-3)\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{1}{2^\alpha} \leq ABC_\alpha(G), \qquad \text{if } \alpha > 0,$$
$$(m-3)\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{1}{2^\alpha} \geq ABC_\alpha(G), \qquad \text{if } -1 \leq \alpha < 0,$$
$$(m-1)\,\frac{4^\alpha}{9^\alpha} + \frac{2^\alpha}{3^\alpha} \geq ABC_\alpha(G), \qquad \text{if } \alpha \leq -1.$$

If $\alpha > -1$, then the equality is attained if and only if $G \in \mathcal{B}_m$. If $\alpha < -1$, then the equality is attained if and only if $G \in \mathcal{C}_m$.

Proof. Item (1) is a direct consequence of Theorems 1 and 2.

Assume now that $m \equiv 1 \pmod 3$, and so, $2m \equiv 2 \pmod 3$. If a 3-regular graph has n vertices and m edges, then handshaking lemma gives $3n = 2m$, a contradiction. Hence, there are no 3-regular graph with m edges. Thus, if G is a graph with n vertices, $m \geq 6$ edges and maximum degree 3, there exists at least a vertex with degree less than 3. Seeking for a contradiction assume that a vertex of G has degree 1 and the other vertices have degree 3. Handshaking lemma gives $3(n-1)+1 = 2m$, and so, $2m \equiv 1 \pmod 3$, a contradiction. Therefore, there are at least two edges incident to a vertex with degree less than 3, and we have

$$\frac{d_u + d_v - 2}{d_u d_v} \geq \frac{1}{2}$$

for these edges. Also,

$$\frac{d_u+d_v-2}{d_ud_v} \geq \frac{2\Delta-2}{\Delta^2} = \frac{4}{9}$$

for every edge. Hence, we have for any $\alpha > 0$

$$ABC_\alpha(G) \geq (m-2)\,\frac{4^\alpha}{9^\alpha} + 2\,\frac{1}{2^\alpha}\,,$$

and the equality holds if and only if G has a vertex with degree 2 and the other vertices with degree 3, i.e., $G \in \mathcal{A}_m$.

If $\alpha < 0$, then we obtain the converse inequality.

Finally, assume that $m \equiv 2 \,(\mathrm{mod}\, 3)$, and so, $2m \equiv 1 \,(\mathrm{mod}\, 3)$. As in the previous case, handshaking lemma gives that there are no 3-regular graph with m edges.

Seeking for a contradiction assume that a graph G has exactly two edges which do not join two vertices with degree 3. Since G is connected, these two edges join vertices with degrees either 2 and 3, or 1 and 3. Therefore, G has either a vertex with degree 2 and the other vertices with degree 3, or two vertices with degree 1 and the other vertices with degree 3. Handshaking lemma gives in both cases $3k + 2 = 2m$ for some integer k, and so, $2m \equiv 2 \,(\mathrm{mod}\, 3)$, a contradiction.

Hence, G has either one or more than two edges not joining two vertices with degree 3.

If G has exactly one edge not joining two vertices with degree 3, then this edge joins vertices with degrees 1 and 3. Thus, $G \in \mathcal{C}_m$ and

$$ABC_\alpha(G) = (m-1)\,\frac{4^\alpha}{9^\alpha} + \frac{2^\alpha}{3^\alpha}\,.$$

If G has at least three edges not joining two vertices with degree 3, then these three edges verify for $\alpha > 0$

$$\Big(\frac{d_u+d_v-2}{d_ud_v}\Big)^\alpha \geq \frac{1}{2^\alpha}\,.$$

Hence,

$$ABC_\alpha(G) \geq (m-3)\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{1}{2^\alpha}\,,$$

and the equality is attained if and only if G has exactly three edges not joining two vertices with degree 3 and these edges have at least an endpoint with degree 2, i.e., $G \in \mathcal{B}_m$.

If $\alpha < 0$, then the converse inequality holds.

We are going to study the function

$$F(\alpha) = \min\left\{(m-1)\,\frac{4^\alpha}{9^\alpha} + \frac{2^\alpha}{3^\alpha}\,,\ (m-3)\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{1}{2^\alpha}\right\}$$
$$= (m-3)\,\frac{4^\alpha}{9^\alpha} + \min\left\{2\,\frac{4^\alpha}{9^\alpha} + \frac{2^\alpha}{3^\alpha}\,,\ 3\,\frac{1}{2^\alpha}\right\}.$$

Let us consider the function

$$H(\alpha) = 2\,\frac{4^\alpha}{9^\alpha} + \frac{2^\alpha}{3^\alpha} - 3\,\frac{1}{2^\alpha}\,.$$

Since $4/9 < 1/2 < 2/3$ and

$$2\log\frac{4}{9} + \log\frac{2}{3} = 5\log\frac{2}{3} > 3\log\frac{1}{2}\,,$$

Corollary 5 gives that there exists a unique negative zero α_0 of H, and $H(\alpha) > 0$ if and only if $\alpha \in (-\infty, \alpha_0) \cup (0, \infty)$. Since $H(-1) = 0$, we have $\alpha_0 = -1$ and

$$(m-1)\,\frac{4^\alpha}{9^\alpha} + \frac{2^\alpha}{3^\alpha} > (m-3)\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{1}{2^\alpha}$$

if and only if $\alpha \in (-\infty, -1) \cup (0, \infty)$. This finishes the proof of item (3). ■

One can easily check that the following holds for the case $m < 6$ (note that $m \geq 3$ when the maximum degree is 3).

Proposition 8. *Let G be a connected graph with $m < 6$ edges and maximum degree 3, and $\alpha \in \mathbb{R}$.*

(1) *If $m = 3$, then G is the star graph S_4 and*

$$ABC_\alpha(G) = 3\,\frac{2^\alpha}{3^\alpha}\,.$$

(2) *If $m = 4$, then*

$$\frac{2^\alpha}{3^\alpha} + 3\,\frac{1}{2^\alpha} \leq ABC_\alpha(G), \qquad \text{if } \alpha > 0,$$
$$\frac{2^\alpha}{3^\alpha} + 3\,\frac{1}{2^\alpha} \geq ABC_\alpha(G), \qquad \text{if } \alpha < 0.$$

The equality in each bound is attained if and only if G is the cycle graph C_3 with an edge attached at a vertex.

(3) *If $m = 5$, then*

$$\frac{4^\alpha}{9^\alpha} + 4\,\frac{1}{2^\alpha} \leq ABC_\alpha(G), \qquad \text{if } \alpha > 0,$$
$$\frac{4^\alpha}{9^\alpha} + 4\,\frac{1}{2^\alpha} \geq ABC_\alpha(G), \qquad \text{if } \alpha < 0.$$

The equality in each bound is attained if and only if G is the complete graph K_4 without an edge.

If $m \geq 11$ is an odd integer, then we denote by $\mathcal{D}_m$ the set of graphs with m edges such that a vertex has degree 2 and the other vertices have degree 4. Since $m-1$ is an even integer (at least 10), there exists a 4-regular graph with $m-1$ edges; if we replace any fixed edge of this graph by a path P_3, then we obtain a graph in $\mathcal{D}_m$ (and so, $\mathcal{D}_m \neq \emptyset$). Obviously, any graph in $\mathcal{D}_m$ can be obtained in this way from a 4-regular graph with $m-1$ edges.

If $m \geq 11$ is an odd integer, then we denote by $\mathcal{E}_m$ the set of graphs with m edges such that two non-adjacent vertices have degree 3 and the other vertices have degree 4. Since $m+1$ is an even integer (grater than 10), there exists a 4-regular graph with $m+1$ edges; if we remove an edge of this graph, then we obtain a graph in $\mathcal{E}_m$. Any graph in $\mathcal{E}_m$ can be obtained in this way from a 4-regular graph with $m+1$ edges.

If $m \geq 11$ is an odd integer, then we denote by $\mathcal{F}_m$ the set of graphs with m edges such that two adjacent vertices have degree 3 and the other vertices have degree 4. If $m \geq 13$, then $m-3$ is an even integer (at least 10), and there exists a 4-regular graph with $m-3$ edges; if we replace two fixed edges of this graph by two paths P_3 and we join by an edge the central vertices of these P_3, then we obtain a graph in $\mathcal{F}_m$. If $m = 11$, then we can obtain a graph in $\mathcal{F}_{11}$ from the complete graph K_4 with $V(K_4) = \{v_1, v_2, v_3, v_4\}$, by adding a path P_3 between v_1 and v_2, another path P_3 between v_3 and v_4, and joining by an edge the central vertices of these P_3.

Theorem 4. *Let G be a connected graph with $m \geq 10$ edges and maximum degree 4, and $\alpha \in \mathbb{R}$.*

(1) *Assume that m is an even integer. Then*

$$m\,\frac{3^\alpha}{8^\alpha} \geq ABC_\alpha(G), \qquad \text{if } \alpha < 0,$$

$$m\,\frac{3^\alpha}{8^\alpha} \leq ABC_\alpha(G), \qquad \text{if } \alpha > 0.$$

The equality in each bound is attained if and only if G is a 4-regular graph.

(2) *Assume that m is an odd integer. Then*

$$\begin{aligned}
(m-2)\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha} &\ge ABC_\alpha(G), && \text{if } \alpha < 0,\\
(m-2)\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha} &\le ABC_\alpha(G), && \text{if } 0 < \alpha \le \alpha_1,\\
(m-5)\,\frac{3^\alpha}{8^\alpha} + 4\,\frac{5^\alpha}{12^\alpha} + \frac{4^\alpha}{9^\alpha} &\le ABC_\alpha(G), && \text{if } \alpha_1 \le \alpha \le \alpha_2,\\
(m-6)\,\frac{3^\alpha}{8^\alpha} + 6\,\frac{5^\alpha}{12^\alpha} &\le ABC_\alpha(G), && \text{if } \alpha \ge \alpha_2,
\end{aligned}$$

where $\alpha_1 \approx 0.33$ is the unique positive solution of the equation

$$3 \cdot 27^\alpha + 2 \cdot 36^\alpha = 4 \cdot 30^\alpha + 32^\alpha,$$

and $\alpha_2 \approx 5.89$ is the unique positive solution of the equation

$$27^\alpha + 32^\alpha = 2 \cdot 30^\alpha.$$

If $\alpha < \alpha_1$, then the equality is attained if and only if $G \in \mathcal{D}_m$. If $\alpha_1 < \alpha < \alpha_2$, then the equality is attained if and only if $G \in \mathcal{F}_m$. If $\alpha > \alpha_2$, then the equality is attained if and only if $G \in \mathcal{E}_m$.

Proof. Item (1) is a direct consequence of Theorems 1 and 2.

Assume now that m is an odd integer. Handshaking Lemma gives that G is not a 4-regular graph, and so, although the bounds in item (1) hold, they are not sharp.

If $G \in \mathcal{D}_m$, then

$$ABC_\alpha(G) = (m-2)\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha}\,.$$

If $G \in \mathcal{E}_m$, then

$$ABC_\alpha(G) = (m-6)\,\frac{3^\alpha}{8^\alpha} + 6\,\frac{5^\alpha}{12^\alpha}\,.$$

If $G \in \mathcal{F}_m$, then

$$ABC_\alpha(G) = (m-5)\,\frac{3^\alpha}{8^\alpha} + 4\,\frac{5^\alpha}{12^\alpha} + \frac{4^\alpha}{9^\alpha}\,.$$

Let us show that if G is a graph with minimum ABC_α when $\alpha > 0$ (respectively, maximum ABC_α when $\alpha < 0$), then $G \in \mathcal{D}_m \cup \mathcal{E}_m \cup \mathcal{F}_m$. In order to do that assume that $\alpha > 0$ (the case $\alpha < 0$ is similar).

Assume that $G \notin \mathcal{D}_m \cup \mathcal{E}_m \cup \mathcal{F}_m$.

Assume that G has a vertex u_1 with degree 2. Since $G \notin \mathcal{D}_m$, there exists an edge e_1 non-incident to u_1 which is incident to a vertex with degree less than 4. Since the two edges incident to u_1 have weight $1/2^\alpha$, e_1 has weight greater than $3^\alpha/8^\alpha$, and every edge has weight at least $3^\alpha/8^\alpha$, we have

$$ABC_\alpha(G) > (m-2)\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha}\,,$$

which is the ABC_α index of the graphs in $\mathcal{D}_m$. Thus, we can assume that each vertex of G with degree less than 4 has degree 1 or 3.

If G has two vertices v_1, v_2 with degree 1, then the edges incident to them have weights at least $2^\alpha/3^\alpha$, and so,

$$ABC_\alpha(G) \ge (m-2)\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{2^\alpha}{3^\alpha} > (m-2)\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha}\,,$$

which is the ABC_α index of the graphs in $\mathcal{D}_m$. Thus, we can assume also that G with has at most a vertex with degree 1.

Note that if G has n vertices and k of them have degree less than 4 ($d_1, \dots, d_k$, respectively), Handshaking Lemma gives

$$4(n-k) + d_1 + \cdots + d_k = 2m \equiv 2 \pmod 4,$$

$$d_1 + \cdots + d_k \equiv 2 \pmod 4.$$

Let V_0 be the set of vertices with degree less than 4, and E_0 the set of edges incident to some vertex in V_0. Let m_1 be the cardinality of the set of edges incident to a vertex in V_0 and to a vertex with degree 4, and m_2 the cardinality of the set of edges incident to two vertices in V_0. Thus, $m_0 = m_1 + m_2$ is the cardinality of E_0. We have

$$m_1 + 2m_2 = \sum_{u \in V_0} d_u.$$

Since m is odd, G is not a 4-regular graph and $m_0 \ge 1$. Also, since G is a connected graph, $m_1 \ge 1$ and so,

$$2m_0 = 2m_1 + 2m_2 \ge 1 + m_1 + 2m_2 = 1 + \sum_{u \in V_0} d_u.$$

Assume that G has exactly a vertex with degree 1 and $r \ge 0$ vertices with degree 3. Thus, $1 + 3r \equiv 2 \pmod 4$ and so, $r \equiv 3 \pmod 4$ and $r \ge 3$. Hence, $2m_0 \ge 2 + 3r \ge 11$ and $m_0 \ge 6$. Since the weight of each edge in E_0 is at least

$$\Big(\frac{3+4-2}{3 \cdot 4}\Big)^\alpha = \frac{5^\alpha}{12^\alpha}\,,$$

and the weight of the edge incident to the vertex with degree 1 is at least

$$\Big(\frac{1+2-2}{1 \cdot 2}\Big)^\alpha = \frac{1}{2^\alpha}\,,$$

we have

$$ABC_\alpha(G) \geq (m-6)\,\frac{3^\alpha}{8^\alpha} + \frac{1}{2^\alpha} + 5\,\frac{5^\alpha}{12^\alpha} > (m-6)\,\frac{3^\alpha}{8^\alpha} + 6\,\frac{5^\alpha}{12^\alpha}\,,$$

which is the ABC_α index of the graphs in $\mathcal{E}_m$.

Assume that G has not vertices with degree 1 and has r vertices with degree 3. Thus, $3r \equiv 2 \pmod 4$ and so, $r \equiv 2 \pmod 4$. Since $G \notin \mathcal{E}_m \cup \mathcal{F}_m$, we have $r > 2$ and then $r \geq 6$. Hence, $2m_0 \geq 1 + 3r \geq 19$ and $m_0 \geq 10$. Since the weight of each edge in E_0 is at least $5^\alpha/12^\alpha$, we have

$$ABC_\alpha(G) \geq (m-10)\,\frac{3^\alpha}{8^\alpha} + 10\,\frac{5^\alpha}{12^\alpha} > (m-6)\,\frac{3^\alpha}{8^\alpha} + 6\,\frac{5^\alpha}{12^\alpha}\,,$$

which is the ABC_α index of the graphs in $\mathcal{E}_m$.

Consequently, if G is a graph with minimum ABC_α when $\alpha > 0$, then $G \in \mathcal{D}_m \cup \mathcal{E}_m \cup \mathcal{F}_m$. A similar argument gives the result if $\alpha < 0$.

Next, we are going to study the function

$$\begin{aligned} F(\alpha) &= \min\left\{(m-2)\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha}\,,\ (m-6)\,\frac{3^\alpha}{8^\alpha} + 6\,\frac{5^\alpha}{12^\alpha}\,,\ (m-5)\,\frac{3^\alpha}{8^\alpha} + 4\,\frac{5^\alpha}{12^\alpha} + \frac{4^\alpha}{9^\alpha}\right\} \\ &= (m-6)\,\frac{3^\alpha}{8^\alpha} + \min\left\{4\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha}\,,\ 6\,\frac{5^\alpha}{12^\alpha}\,,\ \frac{3^\alpha}{8^\alpha} + 4\,\frac{5^\alpha}{12^\alpha} + \frac{4^\alpha}{9^\alpha}\right\}. \end{aligned}$$

Let us consider the functions

$$\begin{aligned} H_0(\alpha) &= 4\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha} - 6\,\frac{5^\alpha}{12^\alpha}\,, \\ H_1(\alpha) &= 3\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha} - 4\,\frac{5^\alpha}{12^\alpha} - \frac{4^\alpha}{9^\alpha}\,, \\ H_2(\alpha) &= \frac{3^\alpha}{8^\alpha} + \frac{4^\alpha}{9^\alpha} - 2\,\frac{5^\alpha}{12^\alpha}\,. \end{aligned}$$

Since $3/8 < 5/12 < 1/2$ and

$$4\log\frac{3}{8} + 2\log\frac{1}{2} < 6\log\frac{5}{12}\,,$$

Corollary 5 gives that there exists a unique positive zero α_0 of H_0, and $H_0(\alpha) > 0$ if and only if $\alpha \in (-\infty, 0) \cup (\alpha_0, \infty)$. Since $H_0(1) = 0$, $\alpha_0 = 1$ and $H_0(\alpha) > 0$ if and only if $\alpha \in (-\infty, 0) \cup (1, \infty)$. Hence,

$$(m-2)\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha} > (m-6)\,\frac{3^\alpha}{8^\alpha} + 6\,\frac{5^\alpha}{12^\alpha}$$

if and only if $\alpha \in (-\infty, 0) \cup (1, \infty)$.

Since $3/8 < 5/12 < 4/9 < 1/2$ and

$$3\log\frac{3}{8} + 2\log\frac{1}{2} < 4\log\frac{5}{12} + \log\frac{4}{9},$$

Lemma 4 gives that there exists a unique positive zero $\alpha_1 \approx 0.33$ of H_1, and $H_1(\alpha) > 0$ if and only if $\alpha \in (-\infty, 0) \cup (\alpha_1, \infty)$. Hence,

$$(m-2)\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha} > (m-5)\,\frac{3^\alpha}{8^\alpha} + 4\,\frac{5^\alpha}{12^\alpha} + \frac{4^\alpha}{9^\alpha}$$

if and only if $\alpha \in (-\infty, 0) \cup (\alpha_1, \infty)$.

Since $3/8 < 5/12 < 4/9$ and

$$\log\frac{3}{8} + \log\frac{4}{9} < 2\log\frac{5}{12},$$

Corollary 5 gives that there exists a unique positive zero $\alpha_2 \approx 5.89$ of H_2, and $H_2(\alpha) > 0$ if and only if $\alpha \in (-\infty, 0) \cup (\alpha_2, \infty)$. Hence,

$$(m-5)\,\frac{3^\alpha}{8^\alpha} + 4\,\frac{5^\alpha}{12^\alpha} + \frac{4^\alpha}{9^\alpha} > (m-6)\,\frac{3^\alpha}{8^\alpha} + 6\,\frac{5^\alpha}{12^\alpha}$$

if and only if $\alpha \in (-\infty, 0) \cup (\alpha_2, \infty)$.

Thus,

$$\max\left\{4\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha},\; 6\,\frac{5^\alpha}{12^\alpha},\; \frac{3^\alpha}{8^\alpha} + 4\,\frac{5^\alpha}{12^\alpha} + \frac{4^\alpha}{9^\alpha}\right\} = 4\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha},$$

for every $\alpha < 0$, and the function

$$u(\alpha) = \min\left\{4\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha},\; 6\,\frac{5^\alpha}{12^\alpha},\; \frac{3^\alpha}{8^\alpha} + 4\,\frac{5^\alpha}{12^\alpha} + \frac{4^\alpha}{9^\alpha}\right\}$$

satisfies

$$u(\alpha) = 4\,\frac{3^\alpha}{8^\alpha} + 2\,\frac{1}{2^\alpha}, \qquad \text{if } 0 < \alpha \le \alpha_1,$$

$$u(\alpha) = \frac{3^\alpha}{8^\alpha} + 4\,\frac{5^\alpha}{12^\alpha} + \frac{4^\alpha}{9^\alpha}, \qquad \text{if } \alpha_1 \le \alpha \le \alpha_2,$$

$$u(\alpha) = 6\,\frac{5^\alpha}{12^\alpha}, \qquad \text{if } \alpha \ge \alpha_2.$$

These facts imply the second item. ■

We deal now with the case $m < 10$ (note that $m \ge 4$ when the maximum degree is 4).

Theorem 5. *Let G be a connected graph with $m < 10$ edges and maximum degree 4, and $\alpha \in \mathbb{R}$.*

(1) *If* $m = 4$, *then* G *is the star graph* S_5 *and*

$$ABC_\alpha(G) = 4\,\frac{3^\alpha}{4^\alpha}\,.$$

(2) *If* $m = 5$, *then*

$$2\,\frac{3^\alpha}{4^\alpha} + 3\,\frac{1}{2^\alpha} \ge ABC_\alpha(G), \qquad \text{if } \alpha < 0,$$

$$2\,\frac{3^\alpha}{4^\alpha} + 3\,\frac{1}{2^\alpha} \le ABC_\alpha(G), \qquad \text{if } \alpha > 0.$$

The equality in each bound is attained if and only if G *is the cycle graph* C_3 *with two edges attached at a vertex.*

(3) *If* $m = 6$, *then*

$$4\,\frac{1}{2^\alpha} + \frac{3^\alpha}{4^\alpha} + \frac{5^\alpha}{12^\alpha} \ge ABC_\alpha(G), \qquad \text{if } \alpha \le \alpha_3,$$

$$6\,\frac{1}{2^\alpha} \ge ABC_\alpha(G), \qquad \text{if } \alpha_3 \le \alpha < 0,$$

$$6\,\frac{1}{2^\alpha} \le ABC_\alpha(G), \qquad \text{if } \alpha > 0,$$

where $\alpha_3 \approx -2.87$ *is the unique negative solution of the equation*

$$9^\alpha + 5^\alpha = 2 \cdot 6^\alpha.$$

If $\alpha < \alpha_3$, *then the equality in the bound is attained if and only if* G *is the graph obtained from the path graphs* P_1 *and* P_3 *by adding a new vertex incident to the four vertices in* P_1 *and* P_3. *If* $\alpha > \alpha_3$, *then the equality in each bound is attained if and only if* G *is the graph obtained from two path graphs* P_2 *by adding a new vertex incident to the four vertices in the two path graphs.*

(4) *If* $m = 7$, *then*

$$6\,\frac{1}{2^\alpha} + \frac{3^\alpha}{8^\alpha} \ge ABC_\alpha(G), \qquad \text{if } \alpha \le \alpha_4,$$

$$3\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{5^\alpha}{12^\alpha} + \frac{3^\alpha}{4^\alpha} \ge ABC_\alpha(G), \qquad \text{if } \alpha_4 \le \alpha < 0,$$

$$3\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{5^\alpha}{12^\alpha} + \frac{3^\alpha}{4^\alpha} \le ABC_\alpha(G), \qquad \text{if } 0 < \alpha \le \alpha_5,$$

$$4\,\frac{1}{2^\alpha} + \frac{4^\alpha}{9^\alpha} + 2\,\frac{5^\alpha}{12^\alpha} \le ABC_\alpha(G), \qquad \text{if } \alpha \ge \alpha_5,$$

where $\alpha_4 \approx -12.48$ *is the unique negative solution of the equation*

$$3 \cdot 32^{\alpha} + 3 \cdot 30^{\alpha} + 54^{\alpha} = 6 \cdot 36^{\alpha} + 27^{\alpha},$$

and $\alpha_5 \approx 0.11$ *is the unique positive solution of the equation*

$$2 \cdot 16^{\alpha} + 15^{\alpha} + 27^{\alpha} = 4 \cdot 18^{\alpha}.$$

If $\alpha < \alpha_4$*, then the equality in the bound is attained if and only if* G *is the graph obtained from the path graph* S_4 *by adding a new vertex incident to the four vertices in* S_4*. If* $\alpha_4 < \alpha < \alpha_5$*, then the equality in each bound is attained if and only if* G *is the graph obtained from the union of the cycle graph* C_3 *and an isolated vertex by adding a new vertex incident to these four vertices. If* $\alpha > \alpha_5$*, then the equality in the bound is attained if and only if* G *is the graph obtained from the path graph* P_4 *by adding a new vertex incident to the four vertices in* P_4*.*

(5) *If* $m = 8$*, then*

$$\begin{aligned} 2\,\frac{1}{2^{\alpha}} + \frac{3^{\alpha}}{8^{\alpha}} + 4\,\frac{5^{\alpha}}{12^{\alpha}} + \frac{4^{\alpha}}{9^{\alpha}} &\geq ABC_{\alpha}(G), && \text{if } \alpha \leq \alpha_6, \\ 4\,\frac{4^{\alpha}}{9^{\alpha}} + 4\,\frac{5^{\alpha}}{12^{\alpha}} &\geq ABC_{\alpha}(G), && \text{if } \alpha_6 \leq \alpha < 0, \\ 4\,\frac{4^{\alpha}}{9^{\alpha}} + 4\,\frac{5^{\alpha}}{12^{\alpha}} &\leq ABC_{\alpha}(G), && \text{if } \alpha > 0, \end{aligned}$$

where $\alpha_6 \approx -2.25$ *is the unique negative solution of the equation*

$$2 \cdot 36^{\alpha} + 27^{\alpha} = 3 \cdot 32^{\alpha}.$$

If $\alpha < \alpha_6$*, then the equality in the bound is attained if and only if* G *is the graph obtained from the complete graph* K_5 *by removing two incident edges. If* $\alpha > \alpha_6$*, then the equality in each bound is attained if and only if* G *is the graph obtained from the complete graph* K_5 *by removing two non-incident edges.*

(6) *If* $m = 9$*, then*

$$\begin{aligned} 3\,\frac{3^{\alpha}}{8^{\alpha}} + 6\,\frac{5^{\alpha}}{12^{\alpha}} &\geq ABC_{\alpha}(G), && \text{if } \alpha < 0, \\ 3\,\frac{3^{\alpha}}{8^{\alpha}} + 6\,\frac{5^{\alpha}}{12^{\alpha}} &\leq ABC_{\alpha}(G), && \text{if } \alpha > 0, \end{aligned}$$

and the equality in each bound is attained if and only if G *is the complete graph* K_5 *with an edge removed.*

Proof. One can easily check that items (1) and (2) hold.

Assume that $m = 9$. Let G_1 be the graph obtained from the complete graph K_5 by removing an edge. We have

$$ABC_\alpha(G_1) = 3\,\frac{3^\alpha}{8^\alpha} + 6\,\frac{5^\alpha}{12^\alpha}\,.$$

Assume that $\alpha > 0$.

Seeking for a contradiction assume that there are four vertices u_1, u_2, u_3, u_4 in G with degree 4. Denote by $v_1, \dots, v_{n-4}$ the other vertices of G, with degrees $d_1, \dots, d_{n-4}$, respectively. Handshaking Lemma gives $18 = 2m = 4 \cdot 4 + d_1 + \cdots + d_{n-4}$ and $d_1 + \cdots + d_{n-4} = 2$. Each vertex u_i has degree 4 and thus, it is incident on at least one vertex in $\{v_1, \dots, v_{n-4}\}$; hence, $d_1 + \cdots + d_{n-4} \ge 4$, a contradiction.

Hence, there are at most three vertices with degree 4. Thus, there are at most three edges incident to two vertices with degree 4; since the other edges have weights at least

$$\Big(\frac{3+4-2}{3 \cdot 4}\Big)^\alpha = \frac{5^\alpha}{12^\alpha}\,,$$

we have

$$ABC_\alpha(G) \ge 3\,\frac{3^\alpha}{8^\alpha} + 6\,\frac{5^\alpha}{12^\alpha}\,,$$

and the equality in this bound is attained if and only if G has three edges incident to two vertices with degree 4 and six edges incident to a vertex with degree 4 and a vertex with degree 3, i.e., $G = G_1$.

If $\alpha < 0$, then we obtain the converse inequality.

These facts give item (6).

Assume that $m = 6$. Let G_2 (respectively, G_3) be the graph obtained from two path graphs P_2 (respectively, the path graphs P_1 and P_3) by adding a new vertex incident to the four vertices in the path graphs. It is easy to check that the extremal graphs are G_2 and/or G_3.

We have

$$ABC_\alpha(G_2) = 6\,\frac{1}{2^\alpha}\,, \qquad ABC_\alpha(G_3) = 4\,\frac{1}{2^\alpha} + \frac{3^\alpha}{4^\alpha} + \frac{5^\alpha}{12^\alpha}\,.$$

We are going to study the functions

$$\min\Big\{6\,\frac{1}{2^\alpha}\,,\, 4\,\frac{1}{2^\alpha} + \frac{3^\alpha}{4^\alpha} + \frac{5^\alpha}{12^\alpha}\Big\} \;\text{ and }\; \max\Big\{6\,\frac{1}{2^\alpha}\,,\, 4\,\frac{1}{2^\alpha} + \frac{3^\alpha}{4^\alpha} + \frac{5^\alpha}{12^\alpha}\Big\}.$$

Let us consider the function

$$H(\alpha) = \frac{3^\alpha}{4^\alpha} + \frac{5^\alpha}{12^\alpha} - 2\,\frac{1}{2^\alpha}\,.$$

Since $5/12 < 1/2 < 3/4$ and

$$\log\frac{3}{4} + \log\frac{5}{12} > 2\log\frac{1}{2}\,,$$

Corollary 5 gives that there exists a unique negative zero $\alpha_3 \approx -2.87$ of H, and $H(\alpha) > 0$ if and only if $\alpha \in (-\infty, \alpha_3) \cup (0, \infty)$. Hence,

$$4\,\frac{1}{2^\alpha} + \frac{3^\alpha}{4^\alpha} + \frac{5^\alpha}{12^\alpha} > 6\,\frac{1}{2^\alpha}$$

if and only if $\alpha \in (-\infty, \alpha_3) \cup (0, \infty)$. These facts give item (3).

Assume that $m = 7$. Let G_4 (respectively, G_5 or G_6) be the graph obtained from the path graph P_4 (respectively, the star graph S_4 or the union of the cycle graph C_3 and an isolated vertex) by adding a new vertex incident to the four vertices in P_4 (respectively, S_4 or the union of C_3 and an isolated vertex). One check that the extremal graphs are G_4, G_5 and/or G_6.

We have

$$ABC_\alpha(G_4) = 4\,\frac{1}{2^\alpha} + \frac{4^\alpha}{9^\alpha} + 2\,\frac{5^\alpha}{12^\alpha}\,,$$

$$ABC_\alpha(G_5) = 6\,\frac{1}{2^\alpha} + \frac{3^\alpha}{8^\alpha}\,,$$

$$ABC_\alpha(G_6) = 3\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{5^\alpha}{12^\alpha} + \frac{3^\alpha}{4^\alpha}\,.$$

We are going to study the functions

$$\min\Big\{4\,\frac{1}{2^\alpha} + \frac{4^\alpha}{9^\alpha} + 2\,\frac{5^\alpha}{12^\alpha}\,,\ 6\,\frac{1}{2^\alpha} + \frac{3^\alpha}{8^\alpha}\,,\ 3\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{5^\alpha}{12^\alpha} + \frac{3^\alpha}{4^\alpha}\Big\},$$

$$\max\Big\{4\,\frac{1}{2^\alpha} + \frac{4^\alpha}{9^\alpha} + 2\,\frac{5^\alpha}{12^\alpha}\,,\ 6\,\frac{1}{2^\alpha} + \frac{3^\alpha}{8^\alpha}\,,\ 3\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{5^\alpha}{12^\alpha} + \frac{3^\alpha}{4^\alpha}\Big\}.$$

Let us consider the function

$$H_1(\alpha) = 3\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{5^\alpha}{12^\alpha} + \frac{3^\alpha}{4^\alpha} - 6\,\frac{1}{2^\alpha} - \frac{3^\alpha}{8^\alpha}\,.$$

Since $3/8 < 5/12 < 4/9 < 1/2 < 3/4$ and

$$3\log\frac{4}{9} + 3\log\frac{5}{12} + \log\frac{3}{4} < 6\log\frac{1}{2} + \log\frac{3}{8}\,,$$

Lemma 7 gives that there exist a unique negative zero $\alpha_4 \approx -12.48$ of H_1 and a unique positive zero $a_1 \approx 1.57$ of H_1, and $H_1(\alpha) > 0$ if and only if $\alpha \in (\alpha_4, 0) \cup (a_1, \infty)$. Hence,

$$3\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{5^\alpha}{12^\alpha} + \frac{3^\alpha}{4^\alpha} > 6\,\frac{1}{2^\alpha} + \frac{3^\alpha}{8^\alpha}$$

if and only if $\alpha \in (\alpha_4, 0) \cup (a_1, \infty)$.

Let us consider the function

$$H_2(\alpha) = 2\,\frac{1}{2^\alpha} + \frac{3^\alpha}{8^\alpha} - \frac{4^\alpha}{9^\alpha} - 2\,\frac{5^\alpha}{12^\alpha}\,.$$

Since $3/8 < 5/12 < 4/9 < 1/2$ and

$$2\log\frac{1}{2} + \log\frac{3}{8} > \log\frac{4}{9} + 2\log\frac{5}{12}\,,$$

Lemma 4 gives that there exists a unique negative zero $a_2 \approx -6.92$ of H_2, and $H_2(\alpha) > 0$ if and only if $\alpha \in (-\infty, a_2) \cup (0, \infty)$. Hence,

$$6\,\frac{1}{2^\alpha} + \frac{3^\alpha}{8^\alpha} > 4\,\frac{1}{2^\alpha} + \frac{4^\alpha}{9^\alpha} + 2\,\frac{5^\alpha}{12^\alpha}$$

if and only if $\alpha \in (-\infty, a_2) \cup (0, \infty)$.

Let us consider the function

$$H_3(\alpha) = 2\,\frac{4^\alpha}{9^\alpha} + \frac{5^\alpha}{12^\alpha} + \frac{3^\alpha}{4^\alpha} - 4\,\frac{1}{2^\alpha}\,.$$

Since $5/12 < 4/9 < 1/2 < 3/4$ and

$$2\log\frac{4}{9} + \log\frac{5}{12} + \log\frac{3}{4} < 4\log\frac{1}{2}\,,$$

Lemma 6 gives that there exists a unique positive zero $\alpha_5 \approx 0.11$ of H_3, and $H_3(\alpha) > 0$ if and only if $\alpha \in (-\infty, 0) \cup (\alpha_5, \infty)$. Hence,

$$3\,\frac{4^\alpha}{9^\alpha} + 3\,\frac{5^\alpha}{12^\alpha} + \frac{3^\alpha}{4^\alpha} > 4\,\frac{1}{2^\alpha} + \frac{4^\alpha}{9^\alpha} + 2\,\frac{5^\alpha}{12^\alpha}$$

if and only if $\alpha \in (-\infty, 0) \cup (\alpha_5, \infty)$. These facts give item (4).

Finally, assume that $m = 8$. Let G_7 (respectively, G_8) be the graph obtained from the complete graph K_5 by removing two non-incident edges (respectively, two incident edges). One can check that the extremal graphs are G_7 and/or G_8.

We have

$$ABC_\alpha(G_7) = 4\,\frac{4^\alpha}{9^\alpha} + 4\,\frac{5^\alpha}{12^\alpha}\,, \qquad ABC_\alpha(G_8) = 2\,\frac{1}{2^\alpha} + \frac{3^\alpha}{8^\alpha} + 4\,\frac{5^\alpha}{12^\alpha} + \frac{4^\alpha}{9^\alpha}\,.$$

We are going to study the functions

$$\min\left\{4\,\frac{4^\alpha}{9^\alpha}+4\,\frac{5^\alpha}{12^\alpha}\,,\;2\,\frac{1}{2^\alpha}+\frac{3^\alpha}{8^\alpha}+4\,\frac{5^\alpha}{12^\alpha}+\frac{4^\alpha}{9^\alpha}\right\},$$

$$\max\left\{4\,\frac{4^\alpha}{9^\alpha}+4\,\frac{5^\alpha}{12^\alpha}\,,\;2\,\frac{1}{2^\alpha}+\frac{3^\alpha}{8^\alpha}+4\,\frac{5^\alpha}{12^\alpha}+\frac{4^\alpha}{9^\alpha}\right\}.$$

Let us consider the function

$$H(\alpha)=2\,\frac{1}{2^\alpha}+\frac{3^\alpha}{8^\alpha}-3\,\frac{4^\alpha}{9^\alpha}\,.$$

Since $3/8<4/9<1/2$ and

$$2\log\frac{1}{2}+\log\frac{3}{8}>3\log\frac{4}{9}\,,$$

Corollary 5 gives that there exists a unique negative zero $\alpha_6\approx-2.25$ of H, and $H(\alpha)>0$ if and only if $\alpha\in(-\infty,\alpha_6)\cup(0,\infty)$. Hence,

$$2\,\frac{1}{2^\alpha}+\frac{3^\alpha}{8^\alpha}+4\,\frac{5^\alpha}{12^\alpha}+\frac{4^\alpha}{9^\alpha}>4\,\frac{4^\alpha}{9^\alpha}+4\,\frac{5^\alpha}{12^\alpha}$$

if and only if $\alpha\in(-\infty,\alpha_6)\cup(0,\infty)$. These facts give item (5). ■

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