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Some Results on Atom–Bond Connectivity Index of Graphs[1]

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Abstract

The atom–bond connectivity (ABC) index of a graph G is defined as

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

where $E(G)$ is the edge set and d_u, d_v are, respectively, the degrees of the vertices u and v in G. In this paper, we present some sharp lower and upper bounds on ABC. In addition, we give a characterization of the maximum and minimum ABC index and the corresponding extremal graphs among all unicyclic graphs, resp. unicyclic chemical graphs.

1 Introduction

The connectivity index, χ, is topological index and it was introduced in 1975 by Milan Randić [3] who has shown this index to reflect molecular branching. However, many physico–chemical properties are dependent on factors rather different than branching. In order to take this into account, but at the same time to keep the spirit of the Randić index, Ernesto Estrada et al. [2] proposed a new topological index, named atom-bond connectivity (ABC) index. It displays an excellent correlation with the heat of formation

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of alkanes [2, 7]. This index is defined as follows:

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

where $E(G)$ is the set of edges and d_u, d_v are the degrees of vertices u and v in G, respectively.

Recall that a connected graph is known as a molecular graph if its maximum degree is at most four. Furtula et al. [1] determined the minimum and maximum values of this index for molecular trees and showed that the star is the unique tree with the maximum ABC index when the number of vertices is given. Kinkar Ch. Das [4] gave the upper and lower bounds for the ABC index of general graphs using parameters such as the number of vertices, edges, pendent vertices and the minimal non-pendent vertices. Recently, Rundan Xing [5] showed the upper bound for ABC index of trees with a perfect matching and fixed maximum degree, respectively. In this paper, we present some sharp lower and upper bounds on ABC index of graphs and give a characterization of the maximum and minimum ABC index and the corresponding extremal graphs among all unicyclic graphs, resp. unicyclic chemical graphs.

2 The lower bound on ABC index

For a connected graph G of order n with m edges, the maximum vertex degree is denoted by Δ, the number of pendent vertices by p and the number of non-pendent edges having at least one end-vertex of degree 2 by l. Denote by x_{ij} the number of edges of G connecting vertices of degree i and j, where $1 \leq i \leq j \leq \Delta$. Denote by n_i the number of vertices with degree i in G for $i = 1, 2, \ldots, \Delta$. Let $\overline{ij} = \sqrt{\frac{i+j-2}{ij}}$. If $V(G)$ is the disjoint union of two non-empty set $V_1(G)$ and $V_2(G)$ such that every vertex in $V_1(G)$ has degree r and every vertex in $V_2(G)$ has degree s $(r > s)$, then G is an $(r, s)-$semiregular graph. The modified second Zagreb index $M_2^*(G)$ is equal to the sum of the products of the reciprocal of the degrees of pairs of adjacent vertices of the underlying molecular graph G, that is, $M_2^*(G) = \sum_{v_i v_j \in E(G)} \frac{1}{d_i d_j}$.

Lemma 2.1. *Let* $\overline{xy} = \sqrt{\frac{x+y-2}{xy}} = \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}}$, *where* $x \geq 1$. *Then* $\overline{2x} = \frac{\sqrt{2}}{2}$.

Proof. The proof is obvious. □

Lemma 2.2. *Let* $\overline{xy} = \sqrt{\frac{x+y-2}{xy}}$. *If* $x \leq y$, *then* $\overline{1x} \leq \overline{1y}$.

Proof. If $x \le y$, then $\frac{y-1}{y} - \frac{x-1}{x} = \frac{y-x}{xy} \ge 0$. Hence $\overline{1y} - \overline{1x} = \sqrt{\frac{y-1}{y}} - \sqrt{\frac{x-1}{x}} \ge 0$. □

Lemma 2.3. ([5]) *Let* $f(x,y) = \sqrt{\frac{x+y-2}{xy}} = \sqrt{\frac{1}{x} + \frac{1}{y} - \frac{2}{xy}}$ *, where* x *,* $y \ge 1$ *. If* $y \ge 2$ *is fixed, then* $f(x,y)$ *is decreasing for* x *.*

Corollary 2.4. *Let* $\overline{xy} = \sqrt{\frac{x+y-2}{xy}}$ *. If* $y \ge 2$ *is fixed, then* $\overline{2y} \ge \overline{xy}$ *for* x $(x \ge 2)$ *.*

Proof. By Lemma 2.3, if $y \ge 2$ is fixed, then $\overline{xy}$ is deceasing for x, where $x \ge 2$. Hence $\overline{2y} \ge \overline{xy}$. □

Let Γ be the class of connected graphs G whose all the edges have at least one end-vertex of degree 2.

Let Γ^* be the class of connected graphs G, which there is at least one edge whose two end-vertices' degree are both Δ, and all other edges have at least one end-vertex of degree 2.

Let Γ^{**} be the class of graph $H = (V, E)$ such that H is connected graph of minimum vertex degree $\delta = 2$ with q edges $v_iv_j \in E(G)$ such that $d_i = d_j = \Delta(\ge 3)$ and the remaining $m - q$ edges $v_iv_j \in E(H)$ such that $d_i = 2$ or $d_j = 2$ or $d_i = d_j = 2$, where Δ is the maximum vertex degree and q is given by $q = \frac{m\Delta}{\Delta+2\sqrt{\Delta-1}}$.

Theorem 2.5. *Let* G *be a simple connected graph with* m *edges, maximum vertex degree* Δ *,* p *pendent vertices. Denote by* l *the number of non-pendent edges having at least one end-vertex of degree* 2 *. Then*

$$ABC(G) \ge \frac{\sqrt{2}(p+l)}{2} + (m-p-l)\frac{\sqrt{2\Delta-2}}{\Delta} .$$

The equality holds if and only if G *is a regular graph or* $G \in \Gamma$ *or* $G \in \Gamma^*$ *or* $G \cong C_n$ *or* $G \cong P_n$ *.*

Proof. By Lemmas 2.1, 2.2, 2.3, we have

$$\begin{aligned} ABC(G) &= \sum_{2\le i\le\Delta} x_{1i}\overline{1i} + \sum_{2\le i\le\Delta} x_{2i}\overline{2i} + \sum_{3\le i\le j\le\Delta} x_{ij}\overline{ij} \\ &\ge (\sum_{2\le i\le\Delta} x_{1i})\overline{12} + (\sum_{2\le i\le\Delta} x_{2i})\overline{2\Delta} + (\sum_{3\le i\le j\le\Delta} x_{ij})\overline{\Delta\Delta} \\ &= \frac{\sqrt{2}(p+l)}{2} + (m-p-l)\frac{\sqrt{2\Delta-2}}{\Delta} . \end{aligned}$$

Now we consider the equality. The equality holding if and only if $x_{1i} = 0$ $(3 \le i \le \Delta)$, $x_{ij} = 0$ $(3 \le i \le j \le \Delta \textit{ and } (i,j) \ne (\Delta,\Delta))$.

Case 1:$\Delta = 2$.

If $x_{22} \neq 0$ and $x_{12} = 0$, then $G \cong C_n$. If $x_{22} \neq 0$ and $x_{12} \neq 0$, then $G \cong P_n$.

If $x_{22} = 0$ and $x_{12} \neq 0$, then $G \cong P_2$.

Case 2:$\Delta \geq 3$.

If $x_{\Delta\Delta} = 0$ and $x_{12}, x_{22}, \ldots, x_{2\Delta}$ are not all zero, then $G \in \Gamma$.

If $x_{\Delta\Delta} \neq 0$ and $x_{12} = x_{22} = \cdots = x_{2\Delta} = 0$, then G is a regular graph.

If $x_{\Delta\Delta} \neq 0$ and $x_{12}, x_{22}, \ldots, x_{2\Delta}$ are not all zero, then $G \in \Gamma^*$. □

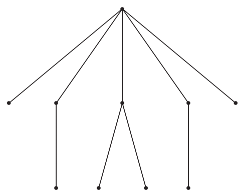
Theorem 2.6. *([4]) Let G be a simple connected graph of order n with m edges, p pendent vertices, maximum vertex degree Δ and minimum non-pendent vertex degree δ_1 . Then*

$$ABC(G) \geq p\sqrt{1 - \frac{1}{\delta_1}} + \frac{\sqrt{4(m-p)(n - 2M_2^*(G) - p(1 - \frac{1}{\Delta}))\sqrt{(\Delta - 1)(\delta_1 - 1)}}}{\sqrt{\Delta\delta_1}(\frac{1}{\Delta}\sqrt{\Delta - 1} + \frac{1}{\delta_1}\sqrt{\delta_1 - 1})} .$$

where $M_2^*(G)$ is the modified second Zagreb index of G . Moreover, the equality holds if and only if G is isomorphic to a $(\Delta, 1)-$semiregular graph or G is isomorphic to a regular graph or $G \in \Gamma^{**}$.

Remark 1. *In this note, Theorem 2.5 has given another bound and it is obviously better than that in Theorem 2.6 in parameters and values, which is an improvement of the bound.*

We give an example as follows:



From the above graph G , we know $M_2^*(G) = \frac{7}{3}$. By Theorem 2.6, we have $ABC(G) \geq \frac{35}{9}\sqrt{2}$. However, by Theorem 2.5, we have $ABC(G) \geq \frac{22}{5}\sqrt{2} > \frac{35}{9}\sqrt{2}$.

Corollary 2.7. *Let G be a simple connected graph with m edges and maximum vertex degree Δ . Then*

$$ABC(G) \geq m\frac{\sqrt{2\Delta - 2}}{\Delta} .$$

The equality holds if and only if G is a regular graph or $G \cong C_n$ or $G \cong P_n$.

Proof. By Theorem 2.5, we have

$$ABC(G) \geq \left(\frac{\sqrt{2}}{2} - \frac{\sqrt{2\Delta - 2}}{\Delta}\right)(p + l) + m\frac{\sqrt{2\Delta - 2}}{\Delta} \geq m\frac{\sqrt{2\Delta - 2}}{\Delta} \, .$$

The equality holds if and only if G is a regular graph or $G \cong C_n$ or $G \cong P_n$.

Corollary 2.8. *Let G^* be a simple connected chemical graph with m edges. Then*

$$ABC(G^*) \geq \frac{\sqrt{6}m}{4} \, .$$

The equality holds if and only if G^* is a $4-$regular graph.

Proof. Since $\Delta \leq 4$, by Corollary 2.7, it is obvious that $ABC(G^*) \geq \frac{\sqrt{6}m}{4}$. The equality holds if and only if G^* is a $4-$regular graph. □

Theorem 2.9. ([4]) *Let G be a simple connected graph with m edges and maximum vertex degree Δ . Then*

$$ABC(G) \geq \frac{2^{\frac{7}{4}} m\sqrt{\Delta - 1}}{\Delta^{\frac{3}{4}}(\sqrt{\Delta} + \sqrt{2})}$$

with equality holding if and only if $G \cong P_n$.

Remark 2. *Since*

$$m\frac{\sqrt{2\Delta - 2}}{\Delta} - \frac{2^{\frac{7}{4}} m\sqrt{\Delta - 1}}{\Delta^{\frac{3}{4}}(\sqrt{\Delta} + \sqrt{2})} = m\sqrt{\Delta - 1}\frac{\sqrt{2}(\Delta^{\frac{1}{4}} - 2^{\frac{1}{4}})^2}{\Delta(\sqrt{\Delta} + \sqrt{2})} \geq 0$$

the lower bound for ABC index of the graph G given in Corollary 2.7 is an improvement of the bound given in Theorem 2.9.

3 The upper bound on ABC index

Let Ψ_1 be the class of connected graphs G , which there is at least one edge whose two end-vertices' degrees are both 3 , and all pendent vertices are adjacent to the maximum degree vertices, and all other edges have at least one end-vertex of degree 2 .

Let Ψ_2 be the class of connected graphs G , whose all pendent vertices are adjacent to the maximum degree vertices and all other edges have at least one end-vertex of degree 2 .

Theorem 3.1. *Let G be a connected graph with m edges, maximum vertex degree Δ, p pendent vertices. Denote by l the number of non-pendent edges having at least one end-vertex of degree 2. Then*

$$ABC(G) \le p\sqrt{1-\frac{1}{\Delta}} + \frac{\sqrt{2}}{2}l + \frac{2(m-p-l)}{3}\ .$$

The equality holds if and only if G is isomorphic to a $3-$regular graph or $G \in \Psi_1$ or $G \in \Psi_2$.

Proof. By Lemmas 2.1, 2.2, 2.3, we have

$$\begin{aligned} ABC(G) &= \sum_{2\le i\le\Delta} x_{1i}\overline{1i} + \sum_{2\le i\le\Delta} x_{2i}\overline{2i} + \sum_{3\le i\le j\le\Delta} x_{ij}\overline{ij} \\ &\le \Big(\sum_{2\le i\le\Delta} x_{1i}\Big)\overline{1\Delta} + \Big(\sum_{2\le i\le\Delta} x_{2i}\Big)\overline{2\Delta} + \Big(\sum_{3\le i\le j\le\Delta} x_{ij}\Big)\overline{33} \\ &= p\sqrt{1-\frac{1}{\Delta}} + \frac{\sqrt{2}}{2}l + \frac{2(m-p-l)}{3}\ . \end{aligned}$$

Now we consider the equality. The equality holding if and only if $x_{1i} = 0$ $(2 \le i \le \Delta-1)$, $x_{ij} = 0$ $(4 \le i \le j \le \Delta)$ and $x_{3i} = 0$ $(4 \le i \le \Delta)$.
Case 1:$x_{33} \ne 0$.
If $x_{1\Delta} = x_{22} = \cdots = x_{2\Delta} = 0$, then we get that G is isomorphic to a 3-regular graph.
If $x_{1\Delta}, x_{22}, \cdots, x_{2\Delta}$ are not all zero, we get $G \in \Psi_1$.
Case 2:$x_{33} = 0$. If $x_{1\Delta}, x_{22}, \cdots, x_{2\Delta}$ are not all zero, then we get $G \in \Psi_2$. □

Lemma 3.2. *([5]) Let i, j and Δ be positive integers with $i \le j \le \Delta$ and $\Delta \ge 3$. Let $h(i,j,\Delta) = 2(\frac{\sqrt{2}}{2} - \sqrt{1-\frac{1}{\Delta}})(\frac{1}{i}+\frac{1}{j}-\frac{1}{2}-\frac{1}{\Delta}) + \sqrt{\frac{i+j-2}{ij}} - \frac{\sqrt{2}}{2}$. Then $h(i,j,\Delta) < 0$ for $(i,j) \ne (1,\Delta),(2,\Delta)$.*

Let Ψ^{**} be the set of connected graphs whose all the edges have one end-vertex of degree Δ and the other end-vertex degree is 1 or 2.

Theorem 3.3. *Let G be a connected graph of order n with m edges and maximum degree Δ, where $2 \le \Delta \le n-1$. Then*

$$ABC(G) \le \sqrt{1-\frac{1}{\Delta}}\Big(2n - m - \frac{2m}{\Delta}\Big) + \sqrt{2}\Big(m + \frac{m}{\Delta} - n\Big)$$

with the equality if and only if $G \in \Psi^{**}$, with $m \equiv 0$ $(mod\ \Delta)$.

Proof. Since G is a graph of order n with m edges and maximum degree Δ, we have

$$\begin{aligned}
n_1 + n_2 + \cdots + n_\Delta &= n \\
n_1 + 2n_2 + \cdots + \Delta n_\Delta &= 2m \\
\sum_{2\le i\le\Delta} x_{1i} &= n_1 \\
\sum_{1\le j\le\Delta \ and \ j\neq i} x_{ij} + 2x_{ii} &= in_i \ (i = 2, 3, \ldots, \Delta) \ .
\end{aligned}$$

Suppose

$$\begin{aligned}
w_1 &= \sum_{2\le i\le\Delta-1} x_{1i} \\
w_2 &= \sum_{1\le j\le\Delta-1 \ and \ j\neq 2} x_{2j} + 2x_{22} \\
w_i &= \sum_{1\le j\le\Delta \ and \ j\neq i} x_{ij} + 2x_{ii} \ (i = 3, 4, \ldots, \Delta) \\
w_\Delta &= \sum_{3\le j\le\Delta-1} x_{j\Delta} + 2x_{\Delta\Delta}
\end{aligned}$$

i. e.,

$$\begin{aligned}
w_1 &= n_1 - x_{1\Delta} \\
w_2 &= 2n_2 - x_{2\Delta} \\
w_i &= in_i \ (i = 3, 4, \cdots, \Delta - 1) \\
w_\Delta &= \Delta n_\Delta - x_{1\Delta} - x_{2\Delta} \ .
\end{aligned}$$

Then we have

$$\begin{aligned}
\sum_{1\le i\le\Delta} w_i &= 2m - 2(x_{1\Delta} + x_{2\Delta}) \\
\sum_{1\le i\le\Delta} \frac{1}{i} w_i &= n - (1 + \frac{1}{\Delta})x_{1\Delta} - (\frac{1}{2} + \frac{1}{\Delta})x_{2\Delta} \ .
\end{aligned}$$

It follows that

$$\begin{aligned}
x_{1\Delta} &= 2n - m - \frac{2m}{\Delta} - \sum_{1\le i\le\Delta} (\frac{2}{i} - \frac{1}{2} - \frac{1}{\Delta})w_i \\
&= 2n - m - \frac{2m}{\Delta} - \sum_{1\le i\le j\le\Delta, \ (i,j)\neq(1,\Delta)(2,\Delta)} (\frac{2}{i} + \frac{2}{j} - 1 - \frac{2}{\Delta})x_{ij} \\
x_{2\Delta} &= 2m + \frac{2m}{\Delta} - 2n + \sum_{1\le i\le\Delta} (\frac{2}{i} - 1 - \frac{1}{\Delta})w_i \\
&= 2m + \frac{2m}{\Delta} - 2n + \sum_{1\le i\le j\le\Delta, \ (i,j)\neq(1,\Delta)(2,\Delta)} (\frac{2}{i} + \frac{2}{j} - 2 - \frac{2}{\Delta})x_{ij} \ .
\end{aligned}$$

Hence by Lemma 3.2, we have

$$\begin{aligned} ABC(G) &= \sqrt{\frac{\Delta-1}{\Delta}}(2n-m-\frac{2m}{\Delta})+\frac{\sqrt{2}}{2}(2m+\frac{2m}{\Delta}-2n) \\ &+ \sum_{1\le i\le j\le \Delta\,,\,(i,j)\neq(1,\Delta)(2,\Delta)} h(i,j,\Delta)x_{ij} \\ &\le \sqrt{\frac{\Delta-1}{\Delta}}(2n-m-\frac{2m}{\Delta})+\sqrt{2}(m+\frac{m}{\Delta}-n)\ . \end{aligned}$$

The equality holds if and only if $x_{ij}=0, where\ (i,j)\neq(1,\Delta),(2,\Delta)$, then $x_{1\Delta}=2n-m-\frac{2m}{\Delta}$, $x_{2\Delta}=2m+\frac{2m}{\Delta}-2n$, with $m\equiv 0\ (mod\ \Delta\ )$, i. e., $G\in\Psi^{**}$. □

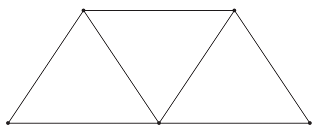
Let Ψ^* be the class of graphs G that are connected, whose vertices are degree of at least two and all the edges have at least one end-vertex of degree 2.

Theorem 3.4. ([4]) *Let G be a simple connected graph of order n with m edges, p pendent vertices, maximum vertex degree Δ and minimum non-pendent vertex degree δ_1. Then*

$$ABC(G)\le p\sqrt{1-\frac{1}{\Delta}}+\frac{m-p}{\delta_1}\sqrt{2(\delta_1-1)}$$

with equality holding if and only if G is isomorphic to a $(\Delta,1)$-semiregular graph or G is isomorphic to a regular graph or $G\in\Psi_2$ or $G\in\Psi^*$.

Remark 3. *Comparing with the upper bound in Theorem 3.4, the bound given in Theorem 3.3 has fewer parameters and is sometimes better than the previous one. So it is significative as a new bound. We give an example as follows.*



From the above graph G, by Theorem 3.4, we have $ABC(G)\le\frac{7\sqrt{2}}{2}$. By Theorem 3.3, we have $ABC(G)\le\frac{15\sqrt{2}-\sqrt{3}}{4}<\frac{7\sqrt{2}}{2}$.

4 On the ABC index of unicyclic graph U and unicyclic chemical graph U^*

A unicyclic graph U is a connected graph in which the number of edges equals the number of vertices. In a unicyclic graph U, the length of the cycle is called its girth, denoted by

g. A unicyclic chemical graph U^* is the unicyclic graph that has no vertex with degree greater than 4.

Let $U_g^*(p)$ be a unicyclic graph, which is obtained from a cycle of length g by attaching p pendent vertices to one vertex of the cycle.

Theorem 4.1. *Let U be a unicyclic connected graph of order n and girth g. Then*

$$ABC(U) \leq (n-g)\sqrt{\frac{n-g+1}{n-g+2}} + \frac{\sqrt{2}}{2}g$$

with the equality if and only if $U \cong U_g^*(n-g)$.

Proof. Since $2 \leq \Delta \leq n-g+2$, by Lemma 3.1, we have

$$\begin{aligned} ABC(U) &\leq p\sqrt{1-\frac{1}{\Delta}} + (\frac{\sqrt{2}}{2} - \frac{2}{3})l + \frac{2(n-p)}{3} \\ &\leq p\sqrt{1-\frac{1}{n-g+2}} + \frac{\sqrt{2}}{2}(n-p) \\ &= p\sqrt{\frac{n-g+1}{n-g+2}} + \frac{\sqrt{2}}{2}(n-p)\,. \end{aligned}$$

Therefore,

$$ABC(U) \leq p\sqrt{\frac{n-g+1}{n-g+2}} + \frac{\sqrt{2}}{2}(n-p)\ (0 \leq p \leq n-g)\,.$$

We consider the function $f(x) = x\sqrt{\frac{n-g+1}{n-g+2}} + \frac{\sqrt{2}}{2}(n-x)$, since $f'(x) \geq 0$, then $ABC(U) \leq (n-g)\sqrt{\frac{n-g+1}{n-g+2}} + \frac{\sqrt{2}}{2}g$. The equality holds if and only if $U \cong U_g^*(n-g)$. □

Corollary 4.2. *Let U be a unicyclic connected graph of order n. Then*

$$ABC(U) \leq (n-3)\sqrt{\frac{n-2}{n-1}} + \frac{3\sqrt{2}}{2}$$

with equality holding if and only if $U \cong U_3^*(n-3)$.

Proof. Since $3 \leq g \leq n$, by Theorem 4.1, we have $ABC(U) \leq (n-g)\sqrt{\frac{n-g+1}{n-g+2}} + \frac{\sqrt{2}}{2}g$. We consider the function $f(x) = (n-x)\sqrt{\frac{n-x+1}{n-x+2}} + \frac{\sqrt{2}}{2}x\ (3 \leq x \leq n)$. Since $f'(x) < 0$, then

$$ABC(U) \leq (n-3)\sqrt{\frac{n-2}{n-1}} + \frac{3\sqrt{2}}{2}$$

with equality holding if and only if $U \cong U_3^*(n-3)$. □

From Corollary 4.2, we conclude that $U_3^*(n-3)$ achieves the maximal ABC index among all unicyclic graphs of order n.

Theorem 4.3. *Let U be a unicyclic connected graph of order n and maximum vertex degree Δ. Then*

$$ABC(U) \geq \frac{n\sqrt{2\Delta - 2}}{\Delta}$$

with equality holding if and only if $U \cong C_n$.

Proof. The proof follows directly from Corollary 2.7. □

Let Φ_1 be the class of unicyclic chemical graphs U^* whose maximum vertex degree is 4 and the vertices of degree 4 are adjacent to the vertices of degree 2 or leaves and the degrees of all other vertices are 2 or 3.

Corollary 4.4. *Let U^* be a unicyclic chemical connected graph of order n with p pendent vertices. Denote by l the number of non-pendent edges having at least one end-vertex of degree 2. Then*

$$ABC(U^*) \leq (\frac{\sqrt{3}}{2} - \frac{2}{3})p + (\frac{\sqrt{2}}{2} - \frac{2}{3})l + \frac{2n}{3}$$

with equality holding if and only if $U^* \in \Phi_1$.

Proof. Since $\Delta \leq 4$, by Theorem 3.1, we have

$$ABC(U^*) \leq p\sqrt{1 - \frac{1}{\Delta}} + \frac{\sqrt{2}l}{2} + \frac{2(n-p-l)}{3} \leq (\frac{\sqrt{3}}{2} - \frac{2}{3})p + (\frac{\sqrt{2}}{2} - \frac{2}{3})l + \frac{2n}{3}\ .$$

The equality holds if and only if $U^* \in \Phi_1$. □

Let Φ_2 be the class of unicyclic chemical connected graphs U^* whose all pendent vertices are adjacent to the vertices of degrees are 4 and all other edges have at least one end-vertex of degree 2.

Theorem 4.5. *Let U^* be the unicyclic chemical connected graph of order n with p pendent vertices. Then*

$$ABC(U^*) \leq \frac{\sqrt{2}}{2}n + \frac{p}{2}(\sqrt{3} - \sqrt{2})$$

with the equality holding if and only if $U^* \in \Phi_2$.

Proof. By Lemmas 2.1, 2.2, 2.3 and Corollary 2.4, we have

$$\begin{aligned}
ABC(U^*) &= x_{12}\overline{12} + x_{13}\overline{13} + x_{14}\overline{14} + x_{22}\overline{22} + x_{23}\overline{23} + x_{24}\overline{24} + x_{33}\overline{33} + x_{34}\overline{34} + x_{44}\overline{44} \\
&= x_{13}\overline{13} + (p - x_{12} - x_{13})\overline{14} + \frac{\sqrt{2}}{2}(x_{12} + x_{22} + x_{23} + x_{24}) + x_{33}\overline{33} + x_{34}\overline{34} \\
&+ (n - p - x_{22} - x_{23} - x_{24} - x_{33} - x_{34})\overline{44} \\
&= p\overline{14} + n\overline{44} - p\overline{44} + (\overline{13} - \overline{14})x_{13} + (\frac{\sqrt{2}}{2} - \overline{14})x_{12} + (\frac{\sqrt{2}}{2} - \overline{44})x_{22} \\
&+ (\frac{\sqrt{2}}{2} - \overline{44})x_{23} + (\frac{\sqrt{2}}{2} - \overline{44})x_{24} + (\overline{33} - \overline{44})x_{33} + (\overline{34} - \overline{44})x_{34} \\
&\leq p\overline{14} + n\overline{44} - p\overline{44} + (\frac{\sqrt{2}}{2} - \overline{44})x_{22} + (\frac{\sqrt{2}}{2} - \overline{44})x_{23} + (\frac{\sqrt{2}}{2} - \overline{44})x_{24} \\
&+ (\overline{33} - \overline{44})x_{33} + (\overline{34} - \overline{44})x_{34} \\
&\leq p\overline{14} + n\overline{44} - p\overline{44} + (\frac{\sqrt{2}}{2} - \overline{44})(x_{22} + x_{23} + x_{24} + x_{33} + x_{34}) \\
&\leq p\overline{14} + n\overline{44} - p\overline{44} + (\frac{\sqrt{2}}{2} - \overline{44})(n - p) \\
&= \frac{\sqrt{2}}{2}n + \frac{p}{2}(\sqrt{3} - \sqrt{2})\ .
\end{aligned}$$

Then $ABC(U^*) \leq \frac{\sqrt{2}}{2}n + \frac{p}{2}(\sqrt{3} - \sqrt{2})$ with the equality if and only if $x_{12} = x_{13} = x_{33} = x_{34} = x_{44} = 0$ and $x_{14}, x_{22}, x_{23}, x_{24}$ are not all zero, that is, $U^* \in \Phi_2$. □

Let $\Gamma^*_{\Delta=4}$ be the class of unicyclic chemical connected graph U^* whose maximum vertex degree is 4 and $U^* \in \Gamma$ or $U^* \in \Gamma^*$.

Theorem 4.6. *Let U^* be a unicyclic chemical connected graph of order n with p pendent vertices. Denote by l the number of non-pendent edges having at least one end-vertex of degree 2. Then*

$$ABC(U^*) \geq (\frac{\sqrt{2}}{2} - \frac{\sqrt{6}}{4})(p + l) + \frac{\sqrt{6}}{4}n$$

with equality holding if and only if $U^* \in \Gamma^*_{\Delta=4}$.

Proof. Since $\Delta \leq 4$, applying Theorem 2.5, we have

$$ABC(U^*) \geq \frac{\sqrt{2}(p + l)}{2} + (n - p - l)\frac{\sqrt{2\Delta - 2}}{\Delta} \geq (\frac{\sqrt{2}}{2} - \frac{\sqrt{6}}{4})(p + l) + \frac{\sqrt{6}}{4}n\ .$$

The equality holds if and only if $x_{13} = x_{14} = x_{33} = x_{34} = 0$ and $x_{12}, x_{22}, x_{23}, x_{24}, x_{44}$ are not all zero and the maximum vertex degree of U^* is 4, that is, $U^* \in \Gamma^*_{\Delta=4}$. □

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