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Some Bounds on General Sum Connectivity Index

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***Abstract*—In this paper, we determine the lower bound for the general sum connectivity index of molecular graphs with $\delta(G) \geq 2$. The extremal molecular structure to reach the lower bound is also presented. Furthermore, we consider the lower bound and extremal molecular graph for triangle-free chemical structures.**

Keywords—theoretical chemistry, molecule graph, general sum connectivity index, triangle-free

I.INTRODUCTION

In theoretical chemistry, drugs and chemical compounds are modeled as graphs where each vertex represents an atom of molecule and covalent bounds between atoms are expressed by edges between the corresponding vertices. The graph obtained from a chemical compounds is often called its molecular graph and can be different structures.

Chemical indices are introduced to reflect certain structural features of organic molecules. Specifically, let *G* be the class of connected molecular graphs, then a topological index can be regarded as a score function *f*: $G \rightarrow \square^{+}$, with this property that $f(G_1) = f(G_2)$ if G_1 and G_2 are isomorphic. There are several vertex distance-based and degree-based indices which introduced to analyze the chemical properties of molecule graph. For instance: Wiener index, PI index, Szeged index, geometric-arithmetic index, atom-bond connectivity index and general sum connectivity index are introduced to test the performance of chemical molecular structures. Several papers contributed to determine these distance-based or degree-based indices of special molecular graph (See Yan et al., [1], Gao et al., [2], Gao and Shi [3], Gao and Wang [4], Xi and Gao [5-6], Xi et al., [7], and Gao et al., [8] for more detail for more detail). The molecular graphs considered in our paper are all simple. The notations and terminologies used but undefined in this paper can be found in Bondy and Mutry [9].

The sum connectivity index ($\chi(G)$) of molecular graph *G* is defined as:

$$\chi(G) = \sum_{uv \in E(G)} (d(u)+d(v))^{-\frac{1}{2}}.$$

Few years ago, Zhou and Trinajstic [10] introduced the general sum connectivity as

$$\chi_k(G) = \sum_{uv \in E(G)} (d(u)+d(v))^{k},$$

where *k* is a real number.

Du et al., [11] reported the maximum value for the general sum connectivity indices of trees with fixed number of vertex, and the corresponding extremal trees for several special real number *k* are determined. Ma and Deng [12] computed the tight lower bounds of the sum connectivity index of cacti. Xing et al., [13] calculated the lower and upper bounds for the sum connectivity indices of tree structure with given numbers of vertices and pendant vertices. Du et al., [14] yielded the minimum sum connectivity indices of trees and unicyclic graphs with fixed number of vertices and matching number, respectively, and the corresponding molecular extremal graphs are deduced. Furthermore, they obtained the first and second minimum sum connectivity indices of the unicyclic graphs with vertex number at least 4. Du et al., [15] derived the minimum and the second minimum values

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of the general sum connectivity indices of unicyclic molecular graphs with non-zero $k \geq -1$ and given vertex number. Moreover, they provided the corresponding molecular extremal graphs. Chen et al., [16] learned the general sum connectivity index of benzenoid systems and phenylenes. Du and Zhou [17] studied the sum connectivity index of bicyclic molecular graphs. Yang et al., [18] reported the computational formulas for calculating the sum connectivity index of polyomino chains. Chen and Li [19] obtained the sharp lower bound of the sum connectivity index for unicyclic molecular graphs with given number of vertex and fixed number of pendent vertices. Farahani [20] deduced the sum connectivity index of special classes of nanotubes. Very recently, Tache [21] obtained the molecular graph with the maximum general sum connectivity index among the connected bicyclic molecular structures with given vertex number and $k \geq 1$.

In this paper, our contributions are two-fold. We first discuss the tight lower bound general sum connectivity index for molecular graphs with $\delta(G) \geq 2$. The sufficient and necessary condition to reach the lower bound is given. Then, we focus on the triangle-tree molecular structures. The corresponding sharp lower bound and extremal structure are presented in triangle-tree setting.

II.MINIMUM GENERAL SUM CONNECTIVITY INDEX OF MOLECULAR GRAPH WITH $\delta(G) \geq 2$ AND $k<0$

For an edge $e=uv$ of a molecular graph G, its general weight is denoted as $(d(u)+d(v))^k$.

Lemma 1. Let e be an edge with maximal general weight in G, and $k<0$. We have

$$\chi_k(G-e) < \chi_k(G).$$

Proof. Let $e=uv$. Since edge uv has maximal general weight in molecular graph G, we get $d(w) \geq d(v)$ for any $w \in N(u)$ and $d(w) \geq d(u)$ for any $w \in N(v)$. Noticing that the function $x^k-(x-1)^k$ is increasing for $x > 1$ and negative real number k, we obtain

$$\chi_k(G) - \chi_k(G-e) = (d(u)+d(v))^k + \sum_{w\in N(u)\backslash\{v\}}((d(u)+d(w))^k-(d(u)+d(w)-1)^k) + \sum_{w\in N(v)\backslash\{u\}}((d(v)+d(w))^k-(d(v)+d(w)-1)^k) \geq$$

$$(d(u)+d(v))^k + (d(u)-1)((d(u)+d(v))^k-(d(u)+d(v)-1)^k) + (d(v)-1)((d(u)+d(v))^k-(d(u)+d(v)-1)^k) =$$

$$(d(u)+d(v)-1)^k-(d(u)+d(v))^k > 0.$$

Hence, we yield the desired result. □

Let $K_{a,b}$ be the complete bipartite molecular graph with a and b vertices in its two partite sets, respectively. For $n \geq 4$, the molecular graph $K_{2,n-2}^*$ is deducedby joining an edge between the two non-adjacent vertices of degree n-2 in $K_{2,n-2}$. By simple calculation, we infer $\chi_k(K_{2,n-2}^*) = f_1(n,k) = (n-1)^k + 2(n-2)(n+1)^k$. We use $\delta(G)$ to denote the minimum degree of the molecular graph G.

Theorem 1. Let G be a molecular graph with vertex number $n \geq 3$ and minimum degree $\delta(G) \geq 2$. Suppose $k<0$. Then $\chi_k(G) \geq f_1(n,k)$ with equality if and only if $G \cong K_{2,n-2}^*$.

Proof. It is not hard to check that the assertion is hold for n=4. Suppose it holds for $4 \leq n' < n$. Then, we show that it also holds for n in the following.

Let *G* be a molecular graph with at least 5 vertices. If $\delta(G) \geq 3$, then according to Lemma 1, the deletion of an edge with maximal general weight gets a graph *G′* of minimal degree at least two such that $\chi_k(G') < \chi_k(G)$. So, in what follows, we only need to verify the result is hold for molecular graph *G* with minimum degree 2.

Case 1. Each pair of adjacent vertices of degree 2 has a common neighbor.

Let u_1 and u_2 be a pair of adjacent vertices with degree 2 in molecular graph *G*, and u_3 is their common neighbor. We immediately get $2 \leq d(u_3) \leq n$-1.

Subcase 1.1. If $d(u_3)$ =2, let G_1=*G*-$\{u_1, u_2, u_3\}$, then $\chi_k(G_1) \geq f_1(n-3,k)$ in view of the induction hypothesis, and $\chi_k(G) = \chi_k(G_1) + 3\cdot 4^k \geq h_1(n-3,k) + 3\cdot 4^k > f_1(n,k)$.

Subcase 1.2. If $d(u_3) \geq 4$, let G_2= *G*-$\{u_1, u_2\}$, then $\chi_k(G_2) \geq f_1(n-2,k)$ in terms of the induction hypothesis. Since $x^k-(x-2)^k$ is increasing for *x* > 2 and *k*<0, we infer

$$\chi_k(G) = \chi_k(G_2) + 4^k + 2(d(u_3)+2)^k + \sum_{v\in N(u_3)\setminus\{u_1,u_2\}}((d(u_3)+d(v))^k-(d(u_3)+d(v)-2)^k) \geq \chi_k(G_2) + 4^k + 2(d(u_3)+2)^k + (d(u_3)-2)((d(u_3)+2)^k-(d(u_3))^k) \geq \chi_k(G_2) + 4^k + 2(d(u_3))^k - 2(d(u_3)+2)^k$$

$$\geq f_1(n-2,k) + 4^k + 2(d(u_3))^k - 2(d(u_3)+2)^k \geq f_1(n-2,k)+4^k+2(n-1)^k - 2(n+1)^k > f_1(n,k).$$

Subcase 1.3. If $d(u_3)$ =3, let u_4 be the neighbor of u_3 in *G* different from u_1 and u_2, where $2 \leq d(u_4) \leq n$−3.

(i) Suppose that $d(u_4)$ =2. Denote by u_5 the neighbor of u_4 in *G* different from u_3, where $2 \leq d(u_5) \leq n$−4. Let G_3 = *G* − $u_4 + u_3u_5$, then $\chi_k(G_3) \geq f_1(n-1,k)$ by the induction hypothesis. Note that $x^k-(x-1)^k$ is decreasing for *x* > 0 and *k*<0.

$$\chi_k(G) = \chi_k(G_3) + 5^k + (d(u_5)+2)^k - (d(u_5)+3)^k$$

$$\geq \chi_k(G_3)+5^k+(n-2)^k-(n-1)^k \geq f_1(n-1,k)+5^k+(n-2)^k-(n-1)^k > f_1(n,k).$$

(ii) Suppose that $3 \leq d(u_4) \leq n$-3. Let G_4 = *G* − $u_1 - u_2 - u_3$, then $\chi_k(G_4) \geq f_1(n-3,k)$ by the induction hypothesis. Note that $(x+2)^k-3(x+1)^k+2(x)^k$ is decreasing for *x* > 0 and *k*<0.

$$\chi_k(G) = \chi_k(G_4) + 4^k + 2\cdot 5^k + (d(u_4)+3)^k + \sum_{v\in N(u_4)\setminus\{u_3\}}((d(u_4)+d(v))^k-(d(u_4)+d(v)-2)^k) \geq \chi_k(G_4) + 4^k + 2\cdot 5^k + (d(u_4)+3)^k + (d(u_4)-1)((d(u_4)+2)^k-(d(u_4)+1)^k) \geq \chi_k(G_4) + 4^k$$

$+2\cdot 5^k+(d(u_4)+3)^k$ - $3(d(u_4)+2)^k+2(d(u_4)+1)^k$

$\geq \chi_k(G_4)+4^k+2\cdot 5^k+n^k$ - $3(n-1)^k+2(n-2)^k \geq$

$f_1(n-3,k)$ + 4^k + $2\cdot 5^k$ + n^k - $3(n-1)^k$ + $2(n-2)^k$ >

$f_1(n,k)$.

Case 2. There is a pair of adjacent vertices of degree two without common neighbor.

Let u_1 and u_2 be a pair of adjacent vertices with degree two in *G* which has no common neighbor. Denote by u_3 the neighbor of u_1 in *G* different from u_2. Let G_5 =*G*− u_1 + u_2u_3, then $\chi_k(G_5) \geq f_1(n-1,k)$ by the induction hypothesis, and $\chi_k(G)$ = $\chi_k(G_5)$ + 4^k ≥ $f_1(n-1,k)+4^k > f_1(n,k)$.

Case 3. There is no pair of adjacent vertices of degree two.

Let *u* be a vertex of degree two with neighbors *v* and *w* in *G*.

Subcase 3.1. $vw \notin E$, where $3\leq d(v) \leq n-2$ and $3 \leq d(w) \leq n-2$. Let G_6 =*G*−*u* + *vw* , then $\chi_k(G_6) \geq f_1(n-1,k)$ by the induction hypothesis. Note that $f(x,y,k)$ = $(x+2)^k$ + $(y+2)^k$ − $(x+y)^k$ ≥ $f(n-2,n-2,k)$ for $3 \leq x \leq n-2$, $3\leq y\leq n-2$ and $k<0$, since $\frac{\partial f}{\partial x} < 0$ and $\frac{\partial f}{\partial y} < 0$.

$\chi_k(G)$ = $\chi_k(G_6)$ + $(d(v)+2)^k$ + $(d(w)+2)^k$ - $(d(v)+d(w))^k$ ≥ $\chi_k(G_6)$ + $f(n-2,n-2,k)$ ≥ $f_1(n-1,k)+2\cdot n^k-(n-2)^k > f_1(n,k)$.

Subcase 3.2. $vw \in E$, where $3\leq d(v) \leq n-1$ and $3 \leq d(w) \leq n-1$. Let G_7 = *G*-*u*, then $\chi_k(G_7) \geq f_1(n-1,k)$ by the induction hypothesis. Note that $g(x,y,k)$ = $(x+y)^k$ + $3(x+1)^k$ + $3(y+1)^k$ - $(x+y-2)^k$ - $3(x+2)^k$ - $3(y+2)^k$ ≥ $g(x-1,y-1,k)$ for $3 \leq x \leq n-1$, $3 \leq y \leq n-1$ and $k<0$, since $\frac{\partial g}{\partial y}(\frac{\partial g}{\partial x})$ <0 and $\frac{\partial g}{\partial x} \leq \frac{\partial g(x,3,k)}{\partial x}$ <0, and $\frac{\partial g}{\partial x}(\frac{\partial g}{\partial y})$ < 0 and $\frac{\partial g}{\partial y} \leq \frac{\partial g(3,y,k)}{\partial y}$ <0.

$$\chi_k(G) = \chi_k(G_7) + (d(v)+2)^k + (d(w)+2)^k - (d(v)+d(w)-2)^k + \sum_{z\in N(v)\setminus\{u,w\}}((d(v)+d(z))^k-(d(v)+d(z)-1)^k) + \sum_{z\in N(w)\setminus\{u,v\}}((d(w)+d(z))^k-(d(w)+d(z)-1)^k)$$

$$\geq \chi_k(G_7) + (d(v)+2)^k + (d(w)+2)^k - (d(v)+d(w)-2)^k + (d(v)-2)((d(v)+2)^k-(d(v)+1)^k) + (d(w)-2)((d(w)+2)^k-(d(w)+1)^k)$$

$$\geq \chi_k(G_7) + (d(v)+d(w))^k + 3(d(v)+1)^k +$$

$3(d(w)+1)^k$ - $(d(v)+d(w)-2)^k$ - $3(d(v)+2)^k$ - $3(d(v)+2)^k$ - $3(d(w)+2)^k$ $\geq$ $\chi_k(G_7)$ + $g(n-1,n-1,k)$ $\geq$ $f_1(n-1,k)$ + $(2n-2)^k$ + $6\cdot n^k$ - $(2n-4)^k$ - $6(n+1)^k$

= $f_1(n,k)$.

with equality if and only if $G\cong K^*_{2,n-2}$.

Hence, the assertion is true for all $n\geq 4$. □

III. A LOWER BOUND FOR THE GENERAL SUM CONNECTITY INDEX OF TRIANGLE-FREE MOLECULAR GRAPH WITH $\delta(G)\geq 2$

In the section, we will give a best possible lower bound for the general sum connectivity index of a triangle-free molecular graph with $\delta(G)$ $\geq$ 2 and characterize the extremal molecular graphs.

Theorem 2. Let *G* be a triangle-free molecular graph of order $n\geq 4$ with $\delta(G)\geq 2$. Assume *k*<0. Then $\chi_k(G)\geq f_2(n,k)=2(n-2)\cdot n^k$ with equality if and only if $G\cong K_{2,n-2}$.

Proof. It is easy to check that the assertion is true for *n*=4. Suppose it holds for $4\leq n'< n$; we next show that it also holds for *n*.

Let *G* be a molecular graph with *n*>4 vertices. If $\delta(G)\geq 3$, then by Lemma 1, the deletion of an edge with maximal general weight yields a graph *G′* of minimal degree at least two such that $\chi_k(G')<\chi_k(G)$. So, we only need to prove the result is true for *G* with $\delta(G)=2$.

Case 1. There exists a vertex *u* of degree two such that the neighbors of *u* have degree at least three.

Let $N(u)=\{u_1, u_2\}$ and $3\leq d(u_i)\leq n-2$ for *i* = 1; 2, then $\delta(G-u)$ $\geq$ 2 and *G*−*u* is triangle-free. $\chi_k(G-u)$ $\geq$ $f_2(n-1,k)$ by the induction hypothesis.

$$\chi_k(G)=\chi_k(G-u)+(d(u_1)+2)^k+(d(u_2)+2)^k+\sum_{v\in N(u_1)\backslash\{u\}}((d(u_1)+d(v))^k-(d(u_1)+d(v)-1)^k)+\sum_{v\in N(u_2)\backslash\{u\}}((d(u_2)+d(v))^k-(d(u_2)+d(v)-1)^k)$$

$$\geq \chi_k(G-u)+(d(u_1)+2)^k+(d(u_2)+2)^k+(d(u_1)-1)((d(u_1)+2)^k-(d(u_1)+1)^k)+(d(u_2)-1)((d(u_2)+2)^k-(d(u_2)+1)^k)$$

$$\geq \chi_k(G-u)+2(d(u_1)+1)^k-2(d(u_1)+2)^k+2(d(u_2)+1)^k-2(d(u_2)+2)^k$$

$$\geq \chi_k(G-u)+2(n-1)^k-2\cdot n^k+2(n-1)^k-2\cdot n^k\geq f_2(n-1,k)+4(n-1)^k-4\cdot n^k=f_2(n,k).$$

with equality if and only if $G\cong K_{2,n-2}$.

Case 2. Every vertex *u* of degree two has a neighbor of degree two in *G*.

Let $N(u)=\{u_1, u_2\}$ and $d(u_1)=2$, $d(u_2)\geq 2$; $N(u_1)=\{u,v\}$.

Subcase 2.1. *v* is not a neighbor of u_2.

Let $G_8=G-u+u_1u_2$, then $\delta(G_8)\geq 2$ and G_8 is triangle-free. $\chi_k(G_8)\geq f_2(n-1,k)$ by the induction hypothesis.

$$\chi_k(G) = \chi_k(G_8) + 4^k \geq f_2(n-1,k) + 4^k > f_2(n,k)$$

.

Subcase 2.2. v is also a neighbor of u_2.

(I) If $d(v) = d(u_2) = 2$, let $G_9 = G - u - v - u_1 - u_2$, then $\delta(G_9) \geq 2$ and G_9 is triangle-free, implying $n \geq 8$. $\chi_k(G_9) \geq f_2(n-4,k)$ by the induction hypothesis.

$$\chi_k(G) = \chi_k(G_9) + 4^{k+1} \geq f_2(n-4,k) + 4^{k+1} > f_2(n,k).$$

(II) If none of v, u_2 has degree two, then $3 \leq d(v) \leq n-3$ and $3 \leq d(u_2) \leq n-3$ since G is triangle-free. Let $G_{10} = G - u - u_1$, then $\delta(G_{10}) \geq 2$ and G_{10} is triangle-free, implying $n \geq 6$. $\chi_k(G_{10}) \geq f_2(n-2,k)$ by the induction hypothesis.

Note that $t(x,y,k) = (x+y)^k - (x+y-2)^k + 3(x+1)^k + 3(y+1)^k - 3(x+2)^k - 2(y+2)^k \geq t(n-3,n-3,k)$

for $3 \leq x \leq n-3$, $3 \leq y \leq n-3$ and $k<0$, since $\frac{\partial}{\partial y}(\frac{\partial t}{\partial x}) < 0$ and $\frac{\partial t}{\partial x} \leq \frac{\partial t(x,3,k)}{\partial x} < 0$ and $\frac{\partial t}{\partial y} < 0$, similarly.

$$\chi_k(G) = \chi_k(G_{10}) + 4^k + (d(v)+2)^k + (d(u_2)+2)^k + (d(v)+d(u_2))^k - (d(v)+d(u_2)-2)^k + \sum_{w \in N(v)\setminus\{u_1,u_2\}} ((d(w)+d(v))^k - (d(w)+d(v)-1)^k) + \sum_{w \in N(u_2)\setminus\{u,v\}} ((d(u_2)+d(w))^k - (d(u_2)+d(w)-1)^k) \geq$$

$$\chi_k(G_{10}) + 4^k + (d(v)+2)^k + (d(u_2)+2)^k + (d(v)+d(u_2))^k - (d(v)+d(u_2)-2)^k$$

$$+ (d(v)-2)((d(v)+2)^k - (d(v)+1)^k) + (d(u_2)-2)((d(u_2)+2)^k - (d(u_2)+1)^k)$$

$$\geq \chi_k(G_{10}) + 4^k + t(d(v), d(u_2), k)$$

$$\geq \chi_k(G_{10}) + 4^k + t(n-3, n-3, k)$$

$$\geq f_2(n-2,k) + 4^k + t(n-3,n-3,k)$$

$$> f_2(n,k).$$

(III) If exactly one of v, u_2 has degree two, without loss of generality, assume $d(u_2) = 2$, then $3 \leq d(v) \leq n-3$ since G is triangle-free.

(i) If $d(v) \geq 4$, let $G_{11} = G - u - u_1 - u_2$, then $\delta(G_{11}) \geq 2$ and G_{11} is triangle-free, implying $n \geq 7$. $\chi_k(G_{11}) \geq f_2(n-3,k)$ by the induction hypothesis.

$$\chi_k(G) = \chi_k(G_{11}) + 1 + 2(d(v)+2)^k + \sum_{w \in N(v)\setminus\{u_1,u_2\}} ((d(w)+d(v))^k - (d(w)+d(v)-2)^k) \geq$$

$$\chi_k(G_{11}) + 1 + 2(d(v)+2)^k + (d(v)-2)((d(v)+2)^k - (d(v))^k)$$

$$\geq \chi_k(G_{11}) + 1 + 2(d(v))^k - 2(d(v)+2)^k$$

$\geq \chi_k(G_{11})$ +1+ $2(n-3)^k$ - $2(n-1)^k$

$\geq f_2(n-3,k)$ +1+ $2(n-3)^k$ - $2(n-1)^k$

$> f_2(n,k)$.

(ii)If $d(v)$ = 3, denote by u_3 the neighbor of v in G different from u_1 and u_2.

(a) If $d(u_3)$ = 2, let u_4 be the neighbor of u_3 in G different from v and G_{12} = $G - u_3 + vu_4$, then $\delta(G_{12}) \geq 2$ and G_{12} is triangle-free. $\chi_k(G_{12}) \geq f_2(n-1,k)$ by the induction hypothesis. And

$$\chi_k(G) = \chi_k(G_{12}) + 5^k + (d(u_4)+2)^k - (d(u_4)+3)^k$$

$$.\geq \chi_k(G_{12}) + 5^k + 4^k - 5^k$$

$$= \chi_k(G_{12}) + 4^k \geq f_2(n-1,k) + 4^k > f_2(n,k).$$

(b) If $d(u_3) \geq 3$, then $d(u_3) \leq n-5$ as G is triangle-free. Let G_{13} = $G-u-v-u_1-u_2$, we have $\delta(G_{13}) \geq 2$ and G_{13} is triangle-free, implying $n \geq 8$. $\chi_k(G_{13}) \geq f_2(n-4,k)$ by the induction hypothesis.

Note that $(x+3)^k$ - $3(x+2)^k$ + $2(x+1)^k$ is decreasing for $x \geq 0$ and k<0.

$$\chi_k(G) = \chi_k(G_{13}) + 1 + 2\cdot 5^k + (d(u_3)+2)^k + \sum_{w\in N(u_3)\setminus\{v\}} ((d(u_3)+d(w))^k - (d(u_3)+d(w)-1)^k)$$

$$\geq \chi_k(G_{13}) + 1 + 2\cdot 5^k + (d(u_3)+2)^k + (d(u_3)-1)((d(u_3)+2)^k - (d(u_3)+1)^k)$$

$$\geq \chi_k(G_{13}) + 1 + 2\cdot 5^k + (d(u_3)+2)^k - 3(d(u_3)+2)^k + 2(d(u_3)+1)^k$$

$$\geq \chi_k(G_{13}) + 1 + 2\cdot 5^k + (n-2)^k - 3(n-3)^k + 2(n-4)^k \geq f_2(n-4,k) + 1 + 2\cdot 5^k + (n-2)^k - 3(n-3)^k + 2(n-4)^k$$

$$> f_2(n,k).$$

The proof of our theorem is completed. □

IV.SUM CONNECTIVITY INDEX OF MOLECULAR GRAPH AND TRIANGLE-FREE MOLECULAR STRUCTURE WITH $\delta(G) \geq 2$

Let $k=-\frac{1}{2}$, we get the following results on sum connectivity index of molecular graph.

Lemma 2. If e is an edge with maximal general weight in G, and k<0, then $\chi(G-e) < \chi(G)$.

Theorem 3. Let G be a molecular graph with vertex number $n \geq 3$ and minimum degree $\delta(G) \geq 2$. Then

$$\chi(G) \geq f_1(n,-\frac{1}{2}) = (n-1)^{-\frac{1}{2}} + 2(n-2)(n+1)^{-\frac{1}{2}}$$

with equality if and only if $G \cong K^*_{2,n-2}$.

Theorem 4. Let G be a triangle-free molecular graph of order $n \geq 4$ with $\delta(G) \geq 2$. Then

$\chi(G) \geq f_2(n,-\frac{1}{2}) = 2(n-2)\cdot n^{-\frac{1}{2}}$ with equality if and only if $G \cong K_{2,n-2}$.

V.CONCLUSION

In this paper, by virtue of molecular graph structural analysis and mathematical derivation, we determine the lower bound of the general harmonic index of molecular graph with $\delta(G) \geq 2$. Furthermore, the lower bound for the general harmonic index of triangle-free molecular graph with $\delta(G) \geq 2$ is deduced.

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