Atom-Bond Sum-Connectivity Index

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Abstract

The branching index (also known as the connectivity index), introduced in Milan Randić's seminal paper [J. Am. Chem. Soc. 97(23) (1975) 6609–6615], is one of the most famous, investigated, and applied among the graph-theoretical molecular descriptors. The atom-bond connectivity (ABC) index [E. Estrada et al., Indian J. Chem. A 37 (1998) 849–855] and the sum-connectivity (SC) index [B. Zhou, N. Trinajstić, J. Math. Chem. 46 (2009) 1252–1270] belong to the class of successful variants of the connectivity index. In the present paper, by amalgamating the core idea of the SC and ABC indices, a new molecular descriptor is put forward – the atom-bond sum-connectivity (ABS) index. The graphs attaining the extreme values of the ABS index are determined over the classes of (molecular) trees and general graphs of a fixed order. A noteworthy property of the ABC index is that it increases when a non-isolated edge is inserted between any two non-adjacent vertices. It is proved that this property holds also for the ABS index.

Keywords: molecular descriptor; topological index; connectivity index; atom-bond connectivity index; sum-connectivity index.

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1 Introduction

All graphs considered in this paper are assumed to be finite. We use standard graph-theoretical notation and terminology. Those used in this paper without being defined, can be found in the books [?, ?, ?, ?].

In chemical graph theory, graph-based molecular structure descriptors are usually referred to as topological indices. The *branching index* (also known as the *connectivity index* or *Randić index*) of a (molecular) graph is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)\, d_G(v)}}\,, \tag{1}$$

where $d_G(w)$ represents the degree of an arbitrary vertex w in G and uv is the edge between the vertices u and v.

This index was introduced by Milan Randić in the mid of 1970s [?], as a measure of the extent of branching in saturated hydrocarbons. It is appropriate to say that the connectivity index is one of the most studied and frequently applied topological indices in chemical graph theory, see the books [?, ?], surveys [?, ?, ?], the recent papers [?, ?, ?, ?], and the references mentioned therein.

The connectivity index was modified in [?] by taking into consideration not only the degree of the end-vertices of the edge uv, but also the degree $d_G(u) + d_G(v) - 2$ of this edge. The resulting index was called *atom-bond connectivity index* (ABC), and is defined as [?]

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)\, d_G(v)}}\,.$$

Note that in the original definition of the ABC index a factor $\sqrt{2}$ was present (see [?]), but it was dropped later.

The reader interested in chemical applications of the ABC index is referred to the papers [?, ?, ?, ?]. We refer the reader interested in its mathematical aspects to the recent review [?] where most of the mathematical properties of the ABC index established till 2021 can be found.

Zhou and Trinajstić [?] proposed another modified version of the connectivity index by replacing in Eq. (??) $d_G(u)\, d_G(v)$ by $d_G(u) + d_G(v)$. They named the resulting index *sum-connectivity index*. The connectivity index and the sum-connectivity index have a strong correlation, and their predicting abilities are almost identical in the majority of situations, see [?, ?, ?]. Details about mathematical aspects of the sum-connectivity index can be found in the survey [?] and in the references quoted therein.

The primary goal of the present paper is to modify the definition of the ABC index by keeping in mind the idea of the sum-connectivity index. We propose to call this new variant of the ABC index (and hence a variant of the connectivity and sum-connectivity indices) the *atom-bond sum-connectivity index*. For a (molecular) graph G, its atom-bond sum-connectivity (ABS) index is defined as

$$ABS(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) + d_G(v)}} = \sum_{uv \in E(G)} \sqrt{1 - \frac{2}{d_G(u) + d_G(v)}} \,.$$

At this point it is worth noting that the so-called *harmonic index* $H(G)$ is [?]

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_G(u) + d_G(v)} \,. \tag{2}$$

In this paper, the graphs that achieve the ABS index's extreme values are found over the classes of all (molecular) trees and general graphs of a fixed order. One of the properties of the ABC index of a (molecular) graph G is that it increases when a non-isolated edge is placed between any two non-adjacent vertices of G (an edge $uv \in E(G)$ is said to be a non-isolated edge if its degree $d_G(u) + d_G(v) - 2$ is non-zero). We now show that this property holds also for the ABS index.

One should note that the ABS index is a special case of the so-called t-index, introduced and studied in [?]. Although, the t-index was studied for several choices of the parameters, none of these include the ABS index.

2 ABS Index of General Trees and Graphs

In this section, some fundamental mathematical properties of the ABS index are established. First, an extremal result for this index concerning graphs (including disconnected ones) is given.

Proposition 1 *If G is a non-trivial graph with n vertices, then*

$$0 \le ABS(G) \le \frac{n\sqrt{(n-2)(n-1)}}{2} \,, \tag{3}$$

where the left equality holds if and only if the maximum degree of G is at most 1, whereas the right equality sign holds if and only if $G \cong K_n$. In other words, among all non-trivial *graphs with n vertices, only the graphs having the maximum degree at most* 1 *possess the minimum value of the ABS index and the complete graph uniquely attains the maximum value of the ABS index.*

Proof: If the size of G is 0, then $ABS(G) = 0$. In what follows, assume that the size of G is at least 1. For every edge $uv \in E(G)$, it holds that

$$\sqrt{1 - \frac{2}{d_G(u) + d_G(v)}} \geq 0\,, \tag{4}$$

with equality if and only if $d_G(u) + d_G(v) = 2$, that is, if and only if $d_G(u) = d_G(v) = 1$. Thus, by applying the summation over all edges on (**??**), one obtains the left inequality of (**??**).

Now, we derive the right inequality of (**??**). For every edge $uv \in E(G)$, it holds that $d_G(u) + d_G(v) \leq 2(n-1)$ with equality if and only if $d_G(u) = d_G(v) = n-1$. Since $n \geq 2$, the last sentence is equivalent to: for every edge $uv \in E(G)$, it holds that

$$\sqrt{1 - \frac{2}{d_G(u) + d_G(v)}} \leq \sqrt{\frac{n-2}{n-1}}\,, \tag{5}$$

with equality if and only if $d_G(u) = d_G(v) = n-1$. Applying the summation over all edges on (**??**) yields

$$ABS(G) \leq \big|E(G)\big|\sqrt{\frac{n-2}{n-1}}\,, \tag{6}$$

which gives the desired inequality because of the fact $\big|E(G)\big| \leq n(n-1)/2$. $\square$

We remark here that (**??**) gives an upper bound on the ABS index of a graph G in terms of its order and size, and this bound is attained if and only if $G \cong K_n$.

Next, we solve the problem of characterizing the trees possessing the maximum and minimum values of the ABS index among all trees of a fixed order. For solving the maximal part of this problem, we derive an upper bound on the ABS index, given in the following proposition.

Proposition 2 *Let $H(G)$ be the harmonic index of the graph G, Eq. (**??**). If G is a graph with m edges, then*

$$ABS(G) \leq \sqrt{m(m - H(G))} \tag{7}$$

with equality if and only if either $m = 0$ or there is a fixed number k such that $d_G(u) + d_G(v) = k$ holds for every edge $uv \in E(G)$.

Proof: For $m = 0$, the result is trivial. Assume that $m \geq 1$. By using the Cauchy–Bunyakovsky–Schwarz inequality, one has

$$\left(\sum_{uv\in E(G)} \sqrt{1-\frac{2}{d_G(u)+d_G(v)}}\right)^2 \leq \left(\sum_{uv\in E(G)} \left(1-\frac{2}{d_G(u)+d_G(v)}\right)\right)\left(\sum_{uv\in E(G)} (1)\right)$$

where the equality holds if and only if there is a fixed number k' such that

$$\sqrt{1-\frac{2}{d_G(u)+d_G(v)}} = k'$$

for every $uv \in E(G)$. □

In the literature, there exist various lower bounds on the harmonic index, see the survey [?]. From each such lower bound and (**??**), one can obtain an upper bound on the ABS index. Zhong [?] proved that for any non-trivial tree T of order n, the inequality $H(T) \geq 2(n-1)/n$ holds with equality if and only if T is the star graph S_n. From this fact and Proposition **??**, the next result follows.

Proposition 3 *If T is a non-trivial tree of order n, then*

$$ABS(T) \leq (n-1)\sqrt{\frac{n-2}{n}} \tag{8}$$

with equality if and only if $T \cong S_n$. In other words, among all non-trivial trees of order $n \geq 4$, the star graph uniquely attains the maximum value of the ABS index.

Proposition **??** follows also from the fact that the ABS index increases when the graph transformation used in the proof of Lemma 2.1 of [?] is applied to a tree of order $n \geq 4$ with maximum degree at most $n-2$.

A pendent path of a graph G is a path $u_1u_2\cdots u_k$ such that $\min\{d_G(u_1), d_G(u_k)\} = 1$, $\max\{d_G(u_1), d_G(u_k)\} \geq 3$, and $d_G(u_i) = 2$ whenever $2 \leq i \leq k-1$. By a branching vertex of a graph, we mean a vertex of degree at least 3. Two pendent paths P and P' of a graph are said to be adjacent if their branching vertices are the same. For a vertex $u \in V(G)$ of a graph G, define $N_G(u) = \{v \in V(G) : \ uv \in E(G)\}$. The members of $N_G(u)$ are called neighbors of u. In the rest of this paper, we take

$$\Phi(x,y) = \sqrt{1-\frac{2}{x+y}},$$

where $\min\{x, y\} \geq 1$.

Next, we prove a result that is crucial for characterizing the tree(s) possessing the minimum value of the ABS index among all trees of a fixed order.

Proposition 4 *If a graph G contains at least one pair of adjacent pendent paths, then there exists at least one graph G' containing no pair of adjacent pendent paths such that $ABS(G) > ABS(G')$.*

Proof: Let $uu_1u_2\cdots u_r$ and $uv_1v_2\cdots v_s$ be two adjacent pendent paths of G, where $d_G(u_r) = d_G(v_s) = 1$. Let G' be the graph formed by deleting the edge uv_1 and inserting the edge u_rv_1. In the following, we prove that $ABS(G) - ABS(G') > 0$; thus, if G' does not contain any pair of adjacent pendent paths then we are done. Otherwise, we repeat the aforementioned graph transformation (on other adjacent pendent paths) unless we arrive at the desired graph.

If $r = s = 1$, then by keeping in mind the fact that $d_G(u) \geq 3$ and that the function Φ defined by

$$\Phi(x, y) = \sqrt{1 - \frac{2}{x + y}}\,,$$

is strictly increasing in both x and y for $x \geq 1$ and $y \geq 1$, one has

$$\begin{aligned} ABS(G) - ABS(G') = & \sum_{w \in N_G(u) \setminus \{u_1, v_1\}} [\Phi(d_G(u), d_G(w)) - \Phi(d_G(u) - 1, d_G(w))] \\ & + \Phi(d_G(u), 1) - \Phi(2, 1) > 0\,, \end{aligned}$$

as desired.

Let exactly one of r and s is equal to 1. Without loss of generality, assume that $r = 1$ and $s \geq 2$. Then,

$$\begin{aligned} ABS(G) - ABS(G') = & \sum_{w \in N_G(u) \setminus \{u_1, v_1\}} [\Phi(d_G(u), d_G(w)) - \Phi(d_G(u) - 1, d_G(w))] \\ & + \Phi(d_G(u), 2) - \Phi(2, 2) > 0\,, \end{aligned}$$

which is again the desired inequality.

In what follows, it is assumed that $r \geq 2$ and $s \geq 2$. Note that the function f defined by $f(x) = 2\Phi(x, 2) - \Phi(x - 1, 2)$, is strictly increasing for $x \geq 3$. Thus,

$$\begin{aligned} ABS(G) - ABS(G') = & \sum_{w \in N_G(u) \setminus \{u_1, v_1\}} [\Phi(d_G(u), d_G(w)) - \Phi(d_G(u) - 1, d_G(w))] \\ & + 2\Phi(d_G(u), 2) - \Phi(d_G(u) - 1, 2) + \Phi(1, 2) - 2\Phi(2, 2) \\ & > [2\Phi(d_G(u), 2) - \Phi(d_G(u) - 1, 2)] + \Phi(1, 2) - 2\Phi(2, 2) \\ & \geq [2\Phi(3, 2) - \Phi(2, 2)] + \Phi(1, 2) - 2\Phi(2, 2) > 0\,. \end{aligned}$$

□

The next result follows immediately from Proposition **??**.

Corollary 5 *Among all trees of order $n \geq 4$, the path graph P_n uniquely attains the minimum value of the ABS index.*

We now observe another notable aspect of the ABS index, concerned with the behavior of the ABS when an edge in a graph is inserted. We give a more general result in this regard.

Proposition 6 *Let u and v be non-adjacent vertices of a graph G, satisfying the inequality $\max\{d_G(u), d_G(v)\} \geq 1$. Denote by $G+uv$ the graph formed by inserting the edge uv to G. Let $\phi(x,y)$ be a non-negative symmetric real-valued function. If the function ϕ is strictly increasing in x for $x \geq 1$ and $y \geq 1$, then*

$$BID_\phi(G+uv) = \sum_{wz \in E(G+uv)} \phi(d_G(w), d_G(z)) > \sum_{wz \in E(G)} \phi(d_G(w), d_G(z)) = BID_\phi(G)\,.$$

Proof: Without loss of generality, we assume that $d_G(u) \geq d_G(v) \geq 0$. If $d_G(v) = 0$, then $d_G(u) \geq 1$ and hence

$$\begin{aligned} BID_\phi(G) - BID_\phi(G+uv) = & \sum_{a \in N_G(u)} [\phi(d_G(u), d_G(a)) - \phi(d_G(u)+1, d_G(a))] \\ & - \phi(d_G(u)+1, 1) < 0\,, \end{aligned}$$

as desired.

If $d_G(v) \geq 1$, then

$$\begin{aligned} BID_\phi(G) - BID_\phi(G+uv) = & \sum_{a \in N_G(u)} [\phi(d_G(u), d_G(a)) - \phi(d_G(u)+1, d_G(a))] \\ & + \sum_{b \in N_G(v)} [\phi(d_G(v), d_G(b)) - \phi(d_G(v)+1, d_G(b))] \\ & - \phi(d_G(u)+1, d_G(v)+1) < 0\,. \end{aligned}$$

□

The next corollary is a direct consequence of Proposition **??**.

Corollary 7 (see [?]) *If u and v are non-adjacent non-isolated vertices of a graph G, then*

$$ISI(G+uv) = \sum_{wz \in E(G+uv)} \frac{d_G(w)\, d_G(z)}{d_G(w)+d_G(z)} > \sum_{wz \in E(G)} \frac{d_G(w)\, d_G(z)}{d_G(w)+d_G(z)} = ISI(G)\,.$$

If $x_1 > x_2 \geq 1$ and $y \geq 1$, then

$$\Phi(x_1, y) = \sqrt{1 - \frac{2}{x_1 + y}} > \sqrt{1 - \frac{2}{x_2 + y}} = \Phi(x_2, y)\,,$$

which implies that the function Φ is strictly increasing in x for $x \geq 1$ and $y \geq 1$. Thus, the next result is another direct consequence of Proposition **??**.

Corollary 8 *If u and v are non-adjacent non-isolated vertices of a graph G, then*

$$ABS(G+uv) > ABS(G)\,.$$

Corollaries **??** and **??** imply the next result.

Proposition 9 *Among all connected graphs of order $n \geq 3$, the path graph P_n and the complete graph K_n uniquely attain the minimum value and maximum value, respectively, of the ABS index.*

3 *ABS* Index of Chemical Trees

In this section, we characterize the trees possessing the maximum and minimum values of the ABS index among all chemical trees of a fixed order n for $n \geq 11$. The solution to the minimal part of this problem follows directly from Corollary **??**.

Corollary 10 *If $n \geq 4$, then among all chemical trees of order n, the path graph P_n uniquely attains the smallest value of the ABS index.*

The remaining part of this section is concerned with the problem of characterizing the trees possessing the greatest value of the ABS index for $n \geq 11$. The number of vertices in a chemical tree T with degree i is denoted by n_i. Let $m_{i,j}$ be the number of edges in T with degrees i and j of their end-vertices. If T is a chemical tree of order n for $n \geq 3$, then

$$ABS(T) = \sum_{1 \leq i \leq j \leq 4} m_{i,j} \sqrt{1 - \frac{2}{i+j}}\,, \tag{9}$$

$$n_1 + n_2 + n_3 + n_4 = n\,, \tag{10}$$

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1)\,, \tag{11}$$

$$\sum_{\substack{1\le i\le 4\\ i\neq j}} m_{j,i} + 2m_{j,j} = j\cdot n_j \quad \text{for } j=1,2,3,4. \tag{12}$$

By solving the system of equations (??)–(??) for the unknowns $m_{1,4}, m_{4,4}, n_1, n_2, n_3, n_4$ and then inserting the values of $m_{4,4}$ and $m_{1,4}$ (these two values are well-known, see for example [?]) into Eq. (??), one gets

$$\begin{aligned} ABS(T) = &\left(\frac{5\sqrt{3}+4\sqrt{15}}{30}\right)n + \left(\frac{4\sqrt{15}-25\sqrt{3}}{30}\right) + \left(\frac{15\sqrt{3}-8\sqrt{15}}{30}\right)m_{1,2}\\ &+\left(\frac{9\sqrt{2}+\sqrt{3}-4\sqrt{15}}{18}\right)m_{1,3} + \left(\frac{15\sqrt{2}-5\sqrt{3}-4\sqrt{15}}{30}\right)m_{2,2}\\ &+\left(\frac{2\sqrt{15}-5\sqrt{3}}{18}\right)m_{2,3} + \left(\frac{5\sqrt{6}-5\sqrt{3}-\sqrt{15}}{15}\right)m_{2,4}\\ &+\left(\frac{30\sqrt{6}-35\sqrt{3}-4\sqrt{15}}{90}\right)m_{3,3} + \left(\frac{45\sqrt{35}-140\sqrt{3}-7\sqrt{15}}{315}\right)m_{3,4}\,. \end{aligned} \tag{13}$$

We take

$$\begin{aligned} \Gamma_{ABS}(T) = &\left(\frac{15\sqrt{3}-8\sqrt{15}}{30}\right)m_{1,2} + \left(\frac{9\sqrt{2}+\sqrt{3}-4\sqrt{15}}{18}\right)m_{1,3}\\ &+\left(\frac{15\sqrt{2}-5\sqrt{3}-4\sqrt{15}}{30}\right)m_{2,2} + \left(\frac{2\sqrt{15}-5\sqrt{3}}{18}\right)m_{2,3}\\ &+\left(\frac{5\sqrt{6}-5\sqrt{3}-\sqrt{15}}{15}\right)m_{2,4} + \left(\frac{30\sqrt{6}-35\sqrt{3}-4\sqrt{15}}{90}\right)m_{3,3}\\ &+\left(\frac{45\sqrt{35}-140\sqrt{3}-7\sqrt{15}}{315}\right)m_{3,4}\\ &\approx -0.16677m_{1,2} - 0.05733m_{1,3} - 0.09797m_{2,2} - 0.05079m_{2,3}\\ &- 0.01905m_{2,4} - 0.02921m_{3,3} - 0.01071m_{3,4}\,. \end{aligned} \tag{14}$$

Then, Eq. (??) can be written as

$$ABS(T) = \left(\frac{1}{2\sqrt{3}} + \frac{2}{\sqrt{15}}\right)n + \left(\frac{2}{\sqrt{15}} - \frac{5}{2\sqrt{3}}\right) + \Gamma_{ABS}(T)\,. \tag{15}$$

For any given integer n greater than 4, it is evident from Eq. (??) that a tree T attains the greatest value of the ABS index among all chemical trees of order n if and only if T possess the greatest value of Γ_{ABS} in the class of chemical trees under consideration. As a consequence, we consider $\Gamma_{ABS}(T)$ instead of $ABS(T)$ in the next lemma.

Lemma 1 *Let T be a chemical tree. The inequality*

$$\Gamma_{ABS}(T) < 2\left(\frac{5\sqrt{6}-5\sqrt{3}-\sqrt{15}}{15}\right)(\approx -0.03811)\,,$$

holds if any of the following conditions holds:
(i) $\max\{m_{1,2}, m_{1,3}, m_{2,2}, m_{2,3}\} \geq 1$,
(ii) $n_2 + n_3 \geq 2$.

Proof: If either $m_{3,3} \geq 2$ or any of $m_{1,2}, m_{1,3}, m_{2,2}, m_{2,3}$ is positive, then the required inequality follows from (??). Assume that $m_{1,2} = m_{2,2} = m_{2,3} = m_{1,3} = 0$, $n_2 + n_3 \geq 2$, and $m_{3,3} \leq 1$. Suppose, to the contrary, that

$$\Gamma_{ABS}(T) \geq 2\left(\frac{5\sqrt{6}-5\sqrt{3}-\sqrt{15}}{15}\right). \tag{16}$$

The equations $m_{3,4} = 3n_3 - 2m_{3,3}$ and $m_{2,4} = 2n_2$ hold because of the system of equations (??). Then by using (??) we have

$$\begin{aligned}\Gamma_{ABS}(T) &= 2\left(\frac{5\sqrt{6}-5\sqrt{3}-\sqrt{15}}{15}\right)n_2 + \left(\frac{30\sqrt{6}-35\sqrt{3}-4\sqrt{15}}{90}\right)m_{3,3}\\ &\quad+\left(\frac{45\sqrt{35}-140\sqrt{3}-7\sqrt{15}}{315}\right)(3n_3-2m_{3,3})\\ &\approx -0.03811n_2 - 0.02921m_{3,3} - 0.01071(3n_3-2m_{3,3})\,. \end{aligned}\tag{17}$$

If $m_{3,3} = 1$, then $n_3 \geq 2$ and hence from (??) it follows that $\Gamma_{ABS}(T)$ attains its maximum value when $n_2 = 0$ and $n_3 = 2$. Thus, (??) yields

$$\begin{aligned}\Gamma_{ABS}(T) &\leq \left(\frac{30\sqrt{6}-35\sqrt{3}-4\sqrt{15}}{90}\right) + 4\left(\frac{45\sqrt{35}-140\sqrt{3}-7\sqrt{15}}{315}\right)\\ &< 2\left(\frac{5\sqrt{6}-5\sqrt{3}-\sqrt{15}}{15}\right)\end{aligned}$$

which contradicts the assumption (**??**).

If $m_{3,3}=0$, then (**??**) gives

$$\Gamma_{ABS}(T) = 2\left(\frac{5\sqrt{6}-5\sqrt{3}-\sqrt{15}}{15}\right)n_2 + 3\left(\frac{45\sqrt{35}-140\sqrt{3}-7\sqrt{15}}{315}\right)n_3$$

$$\approx -0.03811n_2 - 0.03214n_3\,,$$

which together with (**??**) implies that $n_2+n_3 \leq 1$. This is a contradiction to the assumption $n_2+n_3 \geq 2$.

□

The degree set of a graph G is the set of all unequal degrees of vertices of G.

Theorem 2 *For $n \geq 11$, if T is a chemical tree of order n, then*

$$ABS(T) \leq \left(\frac{5\sqrt{3}+4\sqrt{15}}{30}\right)n + \left(\frac{4\sqrt{15}-25\sqrt{3}}{30}\right)$$

$$+ \begin{cases} 2\left(\frac{5\sqrt{6}-5\sqrt{3}-\sqrt{15}}{15}\right) & \text{if } n \equiv 0 \pmod 3 \\ \frac{45\sqrt{35}-140\sqrt{3}-7\sqrt{15}}{105} & \text{if } n \equiv 1 \pmod 3 \\ 0 & \text{if } n \equiv 2 \pmod 3 \end{cases}$$

with equality if and only if the degree set of T is

- $\{1,2,4\}$ *and T contains only one vertex of degree 2, which has neighbors of degree 4 only, whenever $n \equiv 0 \pmod 3$;*
- $\{1,3,4\}$ *and T contains only one vertex of degree 3, which has neighbors of degree 4 only, whenever $n \equiv 1 \pmod 3$;*
- $\{1,4\}$ *whenever $n \equiv 2 \pmod 3$.*

Proof: If any of the inequalities $n_2+n_3 \geq 2$ and $\max\{m_{1,2}, m_{1,3}, m_{2,2}, m_{2,3}\} \geq 1$ holds, then by using Lemma **??** and Eq. (**??**), one has

$$ABS(T) < \left(\frac{5\sqrt{3}+4\sqrt{15}}{30}\right)n + \left(\frac{4\sqrt{15}-25\sqrt{3}}{30}\right) + 2\left(\frac{5\sqrt{6}-5\sqrt{3}-\sqrt{15}}{15}\right)$$

$$< \left(\frac{5\sqrt{3}+4\sqrt{15}}{30}\right)n + \left(\frac{4\sqrt{15}-25\sqrt{3}}{30}\right) + \frac{45\sqrt{35}-140\sqrt{3}-7\sqrt{15}}{105}$$

$$< \left(\frac{5\sqrt{3}+4\sqrt{15}}{30}\right)n + \left(\frac{4\sqrt{15}-25\sqrt{3}}{30}\right),$$

as desired.

In the remaining, assume that $\max\{m_{1,2}, m_{1,3}, m_{2,2}, m_{2,3}\} = 0$ and $n_2 + n_3 \le 1$. Then, $(n_2, n_3) \in \{(0,0), (1,0), (0,1)\}$ and $m_{3,3} = 0$. From Eqs. (**??**) and (**??**), it follows that $n_2 + 2n_3 \equiv n - 2 \pmod 3$, which gives

$$(n_2, n_3) = \begin{cases} (1,0) & \text{if } n \equiv 0 \pmod 3, \\ (0,1) & \text{if } n \equiv 1 \pmod 3, \\ (0,0) & \text{if } n \equiv 2 \pmod 3, \end{cases}$$

which together with the system of equations (**??**) implies that

$$(m_{2,4}, m_{3,4}) = \begin{cases} (2,0) & \text{if } n \equiv 0 \pmod 3, \\ (0,3) & \text{if } n \equiv 1 \pmod 3, \\ (0,0) & \text{if } n \equiv 2 \pmod 3. \end{cases}$$

The required result follows now from Eq. (**??**). □

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