Sombor and KG-Sombor Indices of Benzenoid Systems and Phenlenyes

V.R. Kulli1* and Ivan Gutman2

1Department of Mathematics, Gulbarga University, Kalaburgi (Gulbarga)-585106, India
Email: vrkulli@gmail.com
2Faculty of Science, University of Kragujevac, P.O.Box 60, 34000 Kragujevac, Serbia
Email: gutman@kg.ac.rs
*Corresponding author

Received 20 August 2022; accepted 29 September 2022

Abstract. Let d(v) denote the degree of a vertex v, and d(e) the degree of an edge e. The Sombor index $SO$ is a vertex-degree-based (VDB) topological index, equal to the sum of terms $\sqrt{d(u)^2 + d(v)^2}$ over all pairs of adjacent vertices $u$ and $v$ of the underlying molecular graph. Recently a variant of $SO$ was put forward, the KG-Sombor index, $KG$, equal to the sum of terms $\sqrt{d(u)^2 + d(e)^2}$ where $u$ is an endpoint of the edge $e$. In this paper, we give general expressions for $SO$ and $KG$ of benzenoid systems and phenlenyes.

Keywords: Topological index, Sombor index, KG-Sombor index, degree (of vertex), degree (of edge), benzenoid system, phenylene

AMS Mathematics Subject Classification (2010): 05C05, 05C07, 05C90

1. Introduction

In the current mathematical and chemical literature, several dozens of vertex-degree-based (VDB) graph invariants (usually referred to as “topological indices”) are being considered [1-3].

Their general form is

$$TI(G) = \sum_{uv \in E(G)} F((u), d(v))$$

where $F$ is some function having the property $F(x,y)=F(y,x)$. In Eq. (1) and throughout this paper, $d(u)$ is the degree (= number of first neighbors) of the vertex $u$ of the underlying graph $G$, whereas the summation goes over pairs adjacent of vertices $u,v$, i.e., over the edges $e=uv$ contained in the edge set $E(G)$ of the graph $G$.

An edge of the graph $G$, connecting a vertex of degree $i$ and a vertex of degree $j$, is called an $(i,j)$-edge. The number of such edges will be denoted by $m_{i,j}$. Then Eq. (1) can be written as

$$TI(G) = \sum_{1 \leq i,j \leq 4} F(i, j) m_{i,j}.$$
One of the newly introduced VDB topological indices is the Sombor index [4]

\[ SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2} \]  

(3)

which recently attracted much attention, see [5-9] and the references cited therein. Motivated by the success of the Sombor index, the present authors examined the possibility of including edge degrees, and defined the KG-Sombor index as [10].

\[ KG(G) = \sum_{uv} \sqrt{d(u)^2 + d(e)^2} \]  

(4)

where the summation goes over all pairs of vertices \( u \) and edges \( e \), such that \( u \) is an endpoint of \( e \).

If the other endpoint of the edge \( e \) is the vertex \( v \), then Eq. (4) can be rewritten according to the form of Eq. (1), namely as [10]:

\[ KG(G) = \sum_{u \in G} \left[ \sqrt{d(u)^2 + [d(u) + d(v) - 2]^2} + \sqrt{d(v)^2 + [d(u) + d(v) - 2]^2} \right]. \]  

(5)

Note that in Eq. (5) we use the fact that the degree of an edge \( e=uv \) satisfies the relation \( d(e)=d(u)+d(v)-2 \).

In this paper, we study the Sombor and KG-Sombor indices of benzenoid systems (cf. Fig. 1) and of phenylenes (cf. Fig. 2). These molecular graphs possess only vertices of degree 2 and 3. Consequently, all their edges are of type (2,2), (2,3), and (3,3). Therefore, for benzenoids and phenylenes, Eq. (2) has the following simple form:

\[ TI(G) = F(2,2)m_{2,2} + F(2,3)m_{2,3} + F(3,3)m_{3,3} \]  

(6)

The values of \( F(2,2) \), \( F(2,3) \), and \( F(3,3) \) for the Sombor and KG-Sombor indices follow immediately from Eqs. (3) and (5), respectively. Thus we have:

<table>
<thead>
<tr>
<th>Sombor index</th>
<th>KG-Sombor index</th>
</tr>
</thead>
<tbody>
<tr>
<td>( F(2,2) )</td>
<td>( 2\sqrt{2} )</td>
</tr>
<tr>
<td>( F(2,2) )</td>
<td>( 4\sqrt{2} )</td>
</tr>
<tr>
<td>( F(2,2) )</td>
<td>( 3\sqrt{2} )</td>
</tr>
<tr>
<td>( F(2,3) )</td>
<td>( \sqrt{13} )</td>
</tr>
<tr>
<td>( F(3,3) )</td>
<td>( \sqrt{13} + 3\sqrt{2} )</td>
</tr>
</tbody>
</table>

What remains is no determine the parameters \( m_{2,2} \), \( m_{2,3} \), and \( m_{3,3} \) for benzenoid systems and for phenylenes.

2. On structural features and Sombor indices of benzenoid systems

The structural features of benzenoid systems (= molecular graphs of benzenoid hydrocarbons) have been studied in due detail [11,12], see also [13,14]. Their main topological properties are determined by three parameters, namely:

\( n = \) number of vertices,
\( h = \) number of hexagons, and
\( r = \) number of inlets.

The number of inlets is equal to the number of strings of 3-degree vertices on the boundary of the underlying benzenoid system, for details see [13,14]. The structural detail determined by the sequence 232 is said to be a “fissure”. The features pertaining to the sequences 2332, 23332, and 233332, are referred to as “bay”, “cove”, and “fjord”, respectively, see Figure 1.
Sombor and KG-Sombor Indices of Benzenoid Systems and Phenyles

The edges of a benzenoid system connect either two vertices of degree 2, or two vertices of degree 3, or a vertex of degree 2 with a vertex of degree 3. Thus, its edges are either of type (2,2) or (2,3) or (3,3), noting that all (2,2)- and (2,3)-type edges lie on the boundary. Their numbers are denoted by $m_{2,2}$, $m_{3,3}$, and $m_{2,3}$, respectively, and it is known that [13,14]

$$m_{2,2} = n - 2h - r + 2$$

$$m_{2,3} = 2r$$

$$m_{3,3} = 3h - r - 3$$

Figure 1: A benzenoid system and the structural details on its boundary. It has 4 fissures, one bay, one cove, and one fjord. Thus its number of inlets is $r = 4 + 1 + 1 + 1 = 7$.

Consequently, by using Eq. (6), for any benzenoid system $B$ with $n$ vertices, $h$ hexagons, and $r$ inlets,

$$SO(B) = 2\sqrt{2}(n - 2h - r + 2) + \sqrt{13}(2r) + 3\sqrt{2}(3h - r - 3)$$

$$= 2\sqrt{2}n + 5\sqrt{2}h + (2\sqrt{13} - 5\sqrt{2})r - 5\sqrt{2}$$

$$= 2.828n + 7.071(h - 1) + 0.140r$$

$$KG(B) = 4\sqrt{2}(n - 2h - r + 2) + (\sqrt{13} + 3\sqrt{2})(2r) + 10(3h - r - 3)$$

$$= 4\sqrt{2}n + (30 - 8\sqrt{2})h + (2\sqrt{13} + 2\sqrt{2} - 10)r - (30 - 8\sqrt{2})$$

$$= 5.657n + 18.686(h - 1) + 0.040r$$

3. On structural features and Sombor indices of of phenyles

The molecular graphs of phenylenes consist 6 and 4 membered cycles, so that every 4-membered cycle is adjacent to two 6-membered cycles (or hexagons) and no two hexagons are adjacent. A characteristic example of a phenylene graph is depicted in Figure 2.

Figure 2: A phenylene graph.
A phenylene \( P \) with \( h \) hexagons has \( 6h \) vertices. It has been shown \([13]\) that for a phenylene with \( h \) hexagons and \( r \) inlets,

\[
m_{2,2} = 2h - r + 4
\]
\[
m_{2,3} = 2r
\]
\[
m_{3,3} = 6h - r - 6
\]

from which, in view of Eq. (6), it follows:

\[
SO(P) = 2\sqrt{2}(2h - r + 4) + \sqrt{3}(2r) + 3\sqrt{2}(6h - r - 6)
\]
\[
= 22\sqrt{2}h + (2\sqrt{13} - 5\sqrt{2})r - 10\sqrt{2}
\]
\[
= 31.113h + 0.140r - 14.142
\]

\[
KG(P) = 4\sqrt{2}(2h - r + 4) + (\sqrt{13} + 3\sqrt{2})(2r) + 10(6h - r - 6)
\]
\[
= (60 + 8\sqrt{2})h + (2\sqrt{13} + 2\sqrt{2} - 10)r - (60 - 16\sqrt{2})
\]
\[
= 71.314h + 0.040r - 37.373
\]

Note that the \( r \)-dependence of both Sombor indices is same for benzenoids and phenylenes.

4. Conclusion

In this study, the Sombor and KG-Sombor indices of benzenoid systems and phenylenes are determined. The formulas deduced make it possible to easily calculate the \( SO \)- and \( KG \)-indices for any benzenoid and phenylene graph. In both cases, these depend (in a linearly increasing manner) on the number of vertices, number of hexagons, and number of inlets. The KG-Sombor index is always greater than the Sombor index. In particular, for any benzenoid system \( B \), \( KG(B) > 2SO(B) \).

By comparing Eqs. (3) and (4), it is evident why \( KG \) has the name “Sombor”. The prefix \( KG \) was added to this name, what may be understood as an abbreviated form of Kulli-Gutman.

Acknowledgement. The authors are thankful to the referee for useful comments.

Conflict of interest. The authors declare that they have no conflict of interest.

Authors’ Contributions. All the authors have equal contribution.

REFERENCES

Sombor and KG-Sombor Indices of Benzenoid Systems and Phenylenes