International Journal of Mathematics Trends and Technology
ISSN: 2231 – 5373 /doi:10.14445/22315373/IJMTT-V67I1P503
Volume 67 Issue 1, 17-20, January, 2021

(*a*, *b*) - *KA* Indices of Benzenoid Systems and Phenylenes: The General Case

V.R.Kulli[1], Ivan Gutman[2]

[1]*Department of Mathematics, Gulbarga University, Kalaburgi (Gulbarga)-585106, India*
[2]*Faculty of Science, University of Kragujevac, P.O.Box 60, 34000 Kragujevac, Serbia*

Abstract: *In a recent paper by Kulli, two new vertex-degree-based (VDB) topological indices were put forward, called (a,b)-KA indices, depending on real-number parameters a and b. The majority of hitherto studied VDB indices are special cases of (a,b)-KA indices, for particular values of a and b. In this paper, we give generally valid expressions for (a,b)-KA indices of benzenoid systems and phenylenes, as well as of the respective coindices.*

Keywords:*Topological index, first (a, b)-KA index, second (a, b)-KA index, benzenoid system, phenylene.*

Mathematics Subject Classification:05C05, 05C07, 05C90

I. Introduction

Nowadays there exist several dozens of vertex-degree-based (VDB) topological indices [1,2], proposed in order to serve as molecular structure descriptors. In a recent paper [3], one of the present authors introduced two more VDB indices, named first and second (*a, b*)-*KA* indices, that depend on real-number parameters *a* and *b*. For a molecular graph *G* whose vertex and edge sets are *V(G)* and *E(G)*, respectively, these indices are defined as [3]

$$KA^1_{a,b}(G) = \sum_{uv \in E(G)} \left[d_G(u)^a + d_G(v)^a \right]^b \qquad (1)$$

and

$$KA^2_{a,b}(G) = \sum_{uv \in E(G)} \left[d_G(u)^a \cdot d_G(v)^a \right]^b \qquad (2)$$

where $d_G(u)$ is the degree (= number of first neighbors) of the vertex $u \in V(G)$,and where the summation goes over all pairs *u*,*v* of adjacent vertices of *G*. The respective coindices are defined as [3].

$$\overline{KA}^1_{a,b}(G) = \sum_{uv \notin E(G)} \left[d_G(u)^a + d_G(v)^a \right]^b \qquad (3)$$

$$\overline{KA}^2_{a,b}(G) = \sum_{uv \notin E(G)} \left[d_G(u)^a \cdot d_G(v)^a \right]^b \qquad (4)$$

where the summation goes over all pairs of non-adjacent vertices, assuming that $u \neq v$.

The significance of the *KA*-indices lies on the fact that their special cases, for pertinently chosen values of the parameters *a* and b, coincide with the vast majority of previously considered VDB descriptors. For instance, for $a = b = 1$, $KA^1_{a,b}$ coincides with the half-century old "*first Zagreb index*"[4], whereas for $a = 1$, $b = -½$, $KA^2_{a,b}$ reduces to the classical "*Randić index*"[5]. For $a = 2$, $b = ½$, $KA^1_{a,b}$ is equal to the recently conceived "*Sombor index*" [6]. For more details see in [3].

In [3], the two *KA*-indices and their coindices were calculated for several families of benzenoid hydrocarbons. However, the general case was not solved. In what follows we fill this gap, and offer formulas for $KA^1_{a,b}$, $KA^2_{a,b}$ and their coindices, valid for all benzenoid systems. In order to do this, we need to recall some basic facts of the topological theory of benzenoid molecules [7].

II. Elements of the theory of benzenoid systems

Let *B* be the molecular graph of a benzenoid hydrocarbon. In what follows we refer to it as a "*benzenoid system*"[7].The main topological properties of benzenoid systems are determined by three parameters, namely:

$n = n(B)$, the number of vertices (i.e., number of carbon atoms in the underlying benzenoid molecule),
$h = h(B)$, the number of hexagons (i.e., the number of six-membered rings of the underlying benzenoid molecule),
$r = r(B)$,the number of inlets.

The number of inlets is equal to the number of strings of 3-degree vertices on the boundary of *B*. Namely, when going along the boundary of the benzenoid system *B*, one encounters vertices of degree 2 and of degree 3. The feature 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. For an illustrative example see Figure 1.

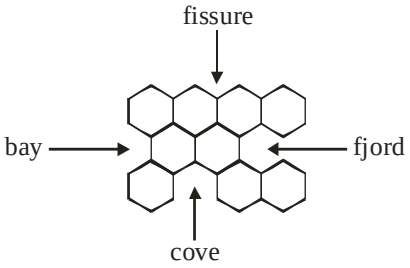


Figure1. A benzenoid system and the features on its boundary. It has 4 fissures, one bay, one cove, and one fjord. Thus its number of inlets is$r$ = 4+1 + 1 + 1 = 7.

All vertices of a benzenoid system *B* are either of degree 2 or of degree 3. Their numbers are

$n_2 = n_2(B) = 2h - 2$
$n_3 = n_3(B) = n - 2h + 2.$

The edges of *B* 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. Their numbers are m_{22}, m_{33}, and m_{23}, respectively. It has been shown [7,8] that

$m_{22} = m_{22}(B) = n - 2h - r + 2$
$m_{33} = m_{33}(B) = 3h - r - 3$
$m_{23} = m_{23}(B) = 2r.$

If we denote by $\bar{m}_{ij}$ the number of pairs of non-adjacent vertices of *B* having degrees *i*and *j*, then

$\bar{m}_{22} = \bar{m}_{22}(B) = \binom{n_2}{2} - m_{22}$
$\bar{m}_{33} = \bar{m}_{33}(B) = \binom{n_3}{2} - m_{33}$
$\bar{m}_{23} = \bar{m}_{23}(B) = n_2 n_3 - m_{23}.$

We see that all structural details of *B*, needed in the subsequent section, are determined by the three fundamental parameters *n, h,* and r.

III. General expressions for (*a, b*)-KA indices of benzenoid systems

Bearing in mind the considerations in the previous section, Eqs. (1), (2), (3), and (4) can be rewritten as

$KA^1_{a,b}(B) = [2^a + 2^a]^b m_{22}(B) + [3^a + 3^a]^b m_{33}(B) + [2^a + 3^a]^b m_{23}(B)$
$KA^2_{a,b}(B) = [2^a \times 2^a]^b m_{22}(B) + [3^a \times 3^a]^b m_{33}(B) + [2^a \times 3^a]^b m_{23}(B)$
$\overline{KA}^1_{a,b}(B) = [2^a + 2^a]^b \bar{m}_{22}(B) + [3^a + 3^a]^b \bar{m}_{33}(B) + [2^a + 3^a]^b \bar{m}_{23}(B)$
$\overline{KA}^2_{a,b}(B) = [2^a \times 2^a]^b \bar{m}_{22}(B) + [3^a \times 3^a]^b \bar{m}_{33}(B) + [2^a \times 3^a]^b \bar{m}_{23}(B)$

from which it follows

$$KA^1_{a,b}(B) = 2^{(a+1)b}(n - 2h - r + 2) + 2^b 3^{ab}(3h - r - 3) + 2(2^a + 3^a)^b r \quad (5)$$

$$KA^2_{a,b}(B) = 2^{2ab}(n - 2h - r + 2) + 3^{2ab}(3h - r - 3) + 2 \cdot 6^{2ab} r \quad (6)$$

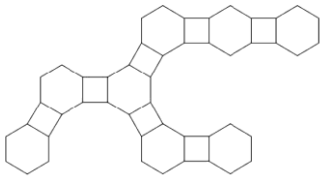
$$\overline{KA}^1_{a,b}(B) = 2^{(a+1)b}[(h-1)(2h-3) - (n - 2h - r + 2)] + 2^b 3^{ab}\left[\frac{1}{2}(n - 2h + 2)(n - 2h + 1) - (3h - r - 3)\right] + 2(2^a + 3^a)^b[(h-1)(n - 2h + 2) - r] \quad (7)$$

$$\overline{KA}^2_{a,b}(B) = 2^{2ab}[(h-1)(2h-3) - (n - 2h - r + 2)] + 3^{2ab}\left[\frac{1}{2}(n - 2h + 2)(n - 2h + 1) - (3h - r - 3)\right] + 2 \cdot 6^{ab}[(h-1)(n - 2h + 2) - r]. \quad (8)$$

These formulas enable the calculation of KA-indices and coindices of any benzenoid system, for which the easily established parameters *n, h, r* are known.

IV. Elements of the theory of phenylenes

Phenylenes are a kind of chemical compounds whose carbon atoms form 6 and 4 members cycles in it. Every 4-membered cycle (or square) is next to two disjoint 6-membered cycles (or hexagons) and no two hexagons are found to be next to each other. By calculation, we obtain that a phenylene *P*has 6*h* vertices and 8*h* – 2 edges, where *h* is the member of hexagons in P[8]. The graph of *P* with 8 hexagons is shown in Figure 2.



PH

Figure 2. Graph of a phenylene *P*.

As for the example of phenylenes, a fissuse, bay, cove, fjord, and logoon are considered in the same manner as the benzenoid systems [8].

All vertices of a phenylene *P* are either of degree 2 or of a degree 3. Their numbers are

$p_2 = p_2(P) = 2h + 4$
$p_3 = p_3(P) = 4h - 4.$

The edge set $E(P)$ can be divided into three partitions [8]:

$e_{22} = e_{22}(P) = 2h - r + 4 = n - 4h - r + 4$
$e_{33} = e_{33}(P) = 6h - r - 6$
$e_{23} = e_{23}(P) = 2r.$

If we denote by $\overline{e}_{ij}$ the number of pairs of non-adjacent vertices of *P* having degree *i* and *j*, then

$$\begin{aligned}\overline{e}_{22}(P) &= \binom{p_2}{2} - e_{22} \\ &= (h+2)(2h+3) - (n-4h-r+r) \\ \overline{e}_{33}(P) &= \binom{p_3}{2} - e_{33} \\ &= (2h-2)(4n-5) - (6h-r-6) \\ \overline{e}_{23}(P) &= p_2 p_3 - e_{23} \\ &= (2h+4)(4h-4) - 2r.\end{aligned}$$

We see that all structural details of *P*, needed in the subsequent section, are computed by the three fundamental parameters *n*, *h*, and *r*.

V. General expressions for (*a*, *b*)-*KA* indices of phenylenes

Bearing in mind the considerations in the previous section, Eqs. (1), (2), (3) and (4) can be rewritten as

$$KA^1_{a,b}(P) = [2^a + 2^a]^b e_{22}(P) + [3^a + 3^a]^b e_{33}(P) + [2^a + 3^a]^b e_{23}(P)$$
$$KA^2_{a,b}(P) = [2^a \times 2^a]^b e_{22}(P) + [3^a \times 3^a]^b e_{33}(P) + [2^a \times 3^a]^b e_{23}(P)$$
$$\overline{KA}^1_{a,b}(P) = [2^a + 2^a]^b \overline{e}_{22}(P) + [3^a + 3^a]^b \overline{e}_{33}(P) + [2^a + 3^a]^b \overline{e}_{23}(P)$$
$$\overline{KA}^2_{a,b}(P) = [2^a \times 2^a]^b \overline{e}_{22}(P) + [3^a \times 3^a]^b \overline{e}_{33}(P) + [2^a \times 3^a]^b \overline{e}_{23}(P)$$

from which it follows.

$$KA^1_{a,b}(P) = 2^{(a+1)b}(n-2h-r+4) + 2^b 3^{ab}(6h-r-6) + 2(2^a + 3^a)^b r$$
$$KA^2_{a,b}(P) = 2^{2ab}(n-4h-r+4) + 3^{2ab}(6h-r+6) + 2 \times 6^{2ab} r$$
$$\overline{KA}^1_{a,b}(P) = 2^{(a+1)b}[(h+2)(2h-3) - (n-4h-r+4)] + 2^b 3^{ab}[(2h+2)(4h-5) - (6h-r-6)]$$
$$+2(2^a + 3^a)^b [(2h+4)(4h-4) - 2r]$$
$$\overline{KA}^2_{a,b}(P) = 2^{2ab}[(h+2)(2h+3) - (n-4h-r+4)] + 3^{2ab}[(2h+2)(4h-5) - (6h-r-6)]$$

$+2\times 6^{ab}\left[(2h-4)(4h-4)-2r\right]$.

These formulas enable the calculation of KA-indices and coindices of any phenylene for which the easily obtained parameters *n, h, r* are known.

VI. Conclusion

In this study, the (*a, b*)-*KA* indices and coindices of benzenoid systems and phenylenes are determined.

VII. References

[1] R.Todeschini and V. Consonni, Molecular Descriptors for Chemoinformatics, Wiley-VCH, Weinheim, (2009).

[2] V.R.Kulli, Graph indices, in: M. Pal, S. Samanta and A. Pal (eds.), Handbook of Research of Advanced Applications of Graph Theory in Modern Society, Global, Hershey, 66-91, (2020).

[3] V.R.Kulli, The (a, b)-KA indices of polycyclic aromatic hydrocarbons and benzenoid systems, International Journal of Mathematical Trends and Technology 65, 115-120, (2019).

[4] I.Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 ,535-538, (1972).

[5] M.Randić, On characterization of molecular branching, J. Am. Chem. Soc. 9 , 6609-6615,(1975).

[6] I.Gutman, Geometric approach to degree-based topological indices: Sombor indices, MATCH Commun. Math. Comput. Chem. 86, 11-16, (2021).

[7] I.Gutman and S. J. Cyvin, Introduction to the Theory of Benzenoid Hydrocarbons, Springer, Berlin, 1989.

[8] J.Rada, O. Araujo and I. Gutman, Randić index of benzenoid systems and phenylenes, Croat. Chem. Acta 74 (2001), 225-235.