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The Connectivity Indices of Regular Graphs[#]

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Explicit formulae for computing the first three vertex- and edge-connectivity indices of regular graphs are given. Formulae for the vertex- and edge-connectivity indices for 2-regular graphs, modeling cycles, are identical because in these graphs the adjacency patterns and the numbers of vertices and edges are the same. In the case of a 3-regular graph, *e.g.,* that of a fullerene, the zero-order and second-order vertex-connectivity indices coincide, and the first three edge-connectivity indices are identical.

Key words: connectivity indices, regular graphs, annulenes, fullerenes

INTRODUCTION

A graph G in which every vertex has the same degree (valency) is called a regular graph.[1,2] If every vertex has degree d, G is called a regular graph of degree d or d-regular graph. Regular graphs can be used to model carbon skeletons of many classes of molecules, *e.g.*, cycles, Platonic and Archimedean molecules, fullerenes, prismane, *etc.* Since regular graphs (and the carbon skeletons of the corresponding molecules) have regular structures, it is possible to express their connectivity indices in a closed form. There are two kinds of connectivity indices: the vertex-connectivity index and the edge-connectivity index.

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DEFINITION OF THE VERTEX-CONNECTIVITY INDEX

The vertex-connectivity index $\chi = \chi(\mathrm{G})$ of a graph G was defined by Randić[3] as a bond-additive quantity:

$$\chi = \sum_{\text{edges}} [d(v_i)\ d(v_j)]^{-1/2} \tag{1}$$

where $d(v_i)$ is the degree of the vertex i, while quantity $[d(v_i)\ d(v_j)]$ can be considered as the weight of the i-j bond.

The vertex-connectivity index can be generalized. The generalization is accomplished by replacing the bond weights $[d(v_i)\ d(v_j)]$ with the path weights $[d(v_i)\ d(v_j)\ ...\ d(v_{\ell+1})]$:[4]

$${}^{\ell}\chi = \sum_{\text{paths}} [d(v_i)\ \mathrm{d}(v_j)\ ...\ d(v_{\ell+1})]^{-1/2}\ . \tag{2}$$

Below we give the definitions of the lowest three vertex-connectivity indices:

(i) The zero-order vertex-connectivity index ${}^0\chi$

$${}^0\chi = \sum_{\text{vertices}} [d(v_i)]^{-1/2}\ . \tag{3}$$

(ii) The first-order vertex-connectivity index ${}^1\chi$ (this index is identical to the original Randić index, see Eq. (1)):

$${}^1\chi = \sum_{\text{edges}} [d(v_i)\ \mathrm{d}(v_j)]^{-1/2}\ . \tag{4}$$

(iii) The second-order vertex-connectivity index ${}^2\chi$

$${}^2\chi = \sum_{\substack{\text{paths of}\\ \text{length two}}} [d(v_i)\ d(v_j)\ d(v_k)]^{-1/2}\ . \tag{5}$$

DEFINITION OF THE EDGE-CONNECTIVITY INDEX

The edge-connectivity index $\varepsilon = \varepsilon(\mathrm{G})$ of a graph G was introduced by Estrada.[5] It is defined similarly to the vertex-connectivity index, but in the definition appear edge-degrees $d(e)$ instead of vertex-degrees $d(v)$:

$$\varepsilon = \sum_{\substack{\text{adjacent}\\ \text{edges}}} [d(e_i)\ d(e_j)]^{-1/2} \tag{6}$$

where $d(e_i)$ is the degree of the edge e_i.

Since an edge e is incident with two vertices v_i and v_j, an edge-degree $d(e)$ of e can be expressed in terms of the corresponding vertex-degrees $d(v_i)$ and $d(v_j)$ as:

$$d(e) = d(v_i) + d(v_j) - 2 \; . \tag{7}$$

Eq. (7) for d-regular graphs, since $d(v_i) = d(v_j) = d(v)$, converts into:

$$d(e) = 2\;[d(v) - 1] \; . \tag{8}$$

Parallel to the handshake lemma which states that the total sum of vertex-degrees equals twice the number of edges:[6]

$$\sum_{i=1}^{V} d(v_i) = 2E \tag{9}$$

it is possible to derive by means of Eq. (8) a related expression for the total sum of edge-degrees in a d-regular graph:

$$\sum_{i=1}^{E} d(e_i) = E\; d(e) = 2\; E\; [d(v) - 1] \tag{10}$$

where E is the number of edges in a graph.

The edge-connectivity index can be generalized similarly as was the vertex-connectivity index:

$$^{\ell}\varepsilon = \sum_{\text{paths}} [d(e_i)\; d(e_j)\; \dots\; d(e_{\ell+1})]^{-1/2} \tag{11}$$

where ℓ is the length of a considered path.

Below we give the definitions of the lowest three edge-connectivity indices:

(i) The zero-order edge-connectivity index $^{0}\varepsilon$

$$^{0}\varepsilon = \sum_{\text{edges}} [d(e_i)]^{-1/2} \; . \tag{12}$$

(ii) The first-order edge-connectivity index $^{1}\varepsilon$

$$^{1}\varepsilon = \sum_{\substack{\text{adjacent}\\ \text{edges}}} [d(e_i)\; d(e_j)]^{-1/2} \; . \tag{13}$$

(iii) The second-order edge-connectivity index $^{2}\varepsilon$

$$^{2}\varepsilon = \sum_{\substack{\text{paths of}\\ \text{three edges}}} [d(e_i)\; d(e_j)\; d(e_k)]^{-1/2} \; . \tag{14}$$

THE VERTEX-CONNECTIVITY INDICES OF d-REGULAR GRAPHS

Eqs. (3)-(5) can be given in a closed form for d-regular graphs. The formulae for vertex-connectivity indices of d-regular graphs can be given in terms of only the number of vertices V and vertex degrees $d(v)$. Note that for regular graphs $\Sigma[d(v_i)] = [d(v_1)] + [d(v_2)] + ... + [d(v_V)] = V\ [d(v)]$.

(i) The zero-order vertex-connectivity index

$$^0\chi = \sum_{\text{vertices}} [d(v_i)]^{-1/2} = V\ [d(v)]^{-1/2} = V/\ [d(v)]^{1/2}\ . \tag{15}$$

(ii) The first-order vertex-connectivity index

$$^1\chi = \sum_{\text{edges}} [d(v_i)\ d(v_j)]^{-1/2} = E\ [d(v)]^{-1} = V/\ 2 \tag{16}$$

where

$$E = V\ d(v)\ /\ 2\ . \tag{17}$$

Formula (16) shows that all non-isomorphic regular graphs with the same number of vertices have identical values of the first-order vertex-connectivity index (or Randić index). This was already observed by Kunz[7] and proved by Estrada.[8]

(iii) The second-order vertex-connectivity index

$$\begin{aligned} ^2\chi &= \sum_{\substack{\text{paths of} \\ \text{length two}}} [d(v_i)\ d(v_j)\ d(v_k)]^{-1/2} = \\ &= V\, d(v)\ [d(v) - 1]\ /\ 2\ d(v)\ [d(v)]^{1/2} \\ &= V\, [d(v) - 1)]\ /\ 2\ [d(v)]^{1/2}\ . \end{aligned} \tag{18}$$

Examples:

(1) Annulenes

Annulenes can be represented by cycles, which are 2-regular graphs, since all vertices in a cycle have degree 2.

(i) The zero-order vertex-connectivity index

$$^0\chi = 0.7071\ V\ . \tag{19}$$

(ii) The first-order vertex-connectivity index

$$^1\chi = 0.5\ V\ . \tag{20}$$

(iii) The second-order vertex-connectivity index

$$^{2}\chi = 0.3536\ V\ . \tag{21}$$

These formulas can be collected as:

$$^{\ell}\chi = d(v)^{-(\ell+1)/2}\ V \tag{22}$$

or

$$^{\ell}\chi = 2^{-(\ell+1)/2}\ V \tag{23}$$

where $\ell = 0, 1,..., N–1$.

(2) Fullerenes

Fullerenes can be represented by 3-regular graphs, since all vertices in fullerenes have degree three. The characteristics of fullerene graphs are discussed, for example, in Ref. 9.

(i) The zero-order vertex-connectivity index

$$^{0}\chi = 0.5774\ V\ . \tag{24}$$

(ii) The first-order vertex-connectivity index

$$^{1}\chi = 0.5\ V\ . \tag{25}$$

(iii) The second-order vertex-connectivity index

It can be straightforwardly shown that $^{0}\chi$ and $^{2}\chi$ are identical for 3-regular graphs.

$$^{0}\chi = {}^{2}\chi = 0.5774\ V\ . \tag{26}$$

These formulas can be collected as:

$$^{\ell}\chi = d(v)^{-(\ell+1)/2}\ P_{\ell} \tag{27}$$

or

$$^{\ell}\chi = 3^{-(\ell+1)/2}\ P_{\ell} \tag{28}$$

where P_{ℓ} is the number of paths of the lenght ℓ. Equations (27) and (28) are valid for all ℓ smaller than the size of the smallest ring. They are similar to Eqs. (22) and (23), where P_{ℓ} is replaced by V because the number of paths of any length in a cycle is equal to the number of vertices. Note that in fullerenes $P_0 = V$, $P_1 = E$ and $P_2 = 3V$.

THE EDGE-CONNECTIVITY INDICES OF d-REGULAR GRAPHS

Eqs. (12)-(14) can also be given in terms of E and $d(e)$ or V and $d(v)$ parameters for d-regular graphs.

(i) The zero-order edge-connectivity index

$$^{0}\varepsilon = \sum_{\text{edges}} [d(e_i)]^{-1/2} = E\ [d(e)]^{-1/2} = E\ /\ [d(e)]^{1/2}\ . \tag{29}$$

This expression alters by means of Eqs. (8) and (17) into somewhat less elegant equation than one above:

$$^{0}\varepsilon = V\, d(v)\ /\ 2\{2\ [d(v) - 1]\}^{1/2}\ . \tag{30}$$

(ii) The first-order edge-connectivity index

$$^{1}\varepsilon = \sum_{\substack{\text{adjacent}\\ \text{edges}}} [d(e_i)\ d(e_j)]^{-1/2} = E\ [d(v) - 1]\ /\ d(e) = \mathrm{E}/2 \tag{31}$$

where Eq. (8) is utilized. Eq. (31) can also be converted by means of Eq. (17) into one containing V and $d(v)$:

$$^{1}\varepsilon = V\, d(v)\ /\ 4\ . \tag{32}$$

Eqs. (31) shows that degeneracy of the first-order edge-connectivity index will appear for regular graphs with identical number of edges.

(iii) The second-order edge-connectivity index

$$^{2}\varepsilon = \sum_{\substack{\text{path of}\\ \text{three edges}}} [d(e_i)\ d(e_j)\ d(e_k)]^{-1/2} = P_3\ /\ d(e)\ [d(e)]^{1/2} \tag{33}$$

or

$$^{2}\varepsilon = P_3\ /\ 2\ [d(v) - 1]\ \{2[d(v) - 1]\}^{1/2} \tag{34}$$

where P_3 is the number of paths consisting of three edges.

The P_3-values can be calculated from the formula:

$$P_3 = E\ [d(e)\ /\ 2]^2 - 3\ C_3$$

$$= \mathrm{V}\ d(v)\ [d(v) - 1]^2\ /\ 2 - 3\ C_3 \tag{35}$$

where C_3 stands for the number of three-membered cycles in d-regular graphs. For example, in the case of the tetrahedral graph (representing the tetrahedron and possessing 4 C_3-cycles) there are 12 distinct P_3 paths.[10]

Examples:

(1) Annulenes

The edge-degrees in annulenes are equal to 2.

(i) The zero-order edge-connectivity index

$$^{0}\varepsilon = 0.7071\ E\ . \tag{36}$$

This index is identical to the zero-order vertex-connectivity index, because in cycles $V = E$ and $d(v) = d(e)$.

(ii) The first-order edge-connectivity index

$$^{1}\varepsilon = 0.5\ E\ . \tag{37}$$

This index is obviously identical to the first-order vertex-connectivity index.

(iii) The second-order edge-connectivity index

$$^{2}\varepsilon = 0.3536\ E\ . \tag{38}$$

Note that in cycles C_V, P_3 = the size of the cycle, V. Since for cycles $E = V$, Eqs. (21) and (38) are identical. Therefore, for annulenes the vertex- and the edge-connectivity indices are identical. This is an extension of the result that was also established by Estrada[8] for the first-order vertex-connectivity index.

Therefore, in general $^{\ell}\varepsilon$ for annulenes can be also computed by means of Eq. (23).

(2) Fullerenes

The edge-degrees in fullerenes are equal to 4.

(i) The zero-order edge-connectivity index

$$^{0}\varepsilon = 0.5\ E \tag{39}$$

or

$$^{0}\varepsilon = 0.75\ V\ . \tag{40}$$

Note that in fullerenes $E = 3\ V/2$. Eqs. (24) and (40) show that the zero-order vertex-connectivity index and the zero-order edge-connectivity index do not coincide for a fullerene.

(ii) The first-order edge-connectivity index

$$^{1}\varepsilon = 0.5\ E \tag{41}$$

or

$$^{1}\varepsilon = 0.75\ V\ . \tag{42}$$

(iii) The second-order edge-connectivity index

$$^{2}\varepsilon = (4E - 3\ C_3)\ /\ 8 \tag{43}$$

or

$$^{2}\varepsilon = 3\ (2V - C_3)\ /\ 8\ . \tag{44}$$

In 3-regular graphs modeling fullerenes, which are ordinarily made up from five- and six-membered rings, vertex- and edge-degrees, $d(v) = 3$ and $d(e) = 4$, are the same for the whole series, whilst there are no three-membered cycles present ($C_3 = 0$). Thus, Eqs. (43) and (44) convert into:

$$^{2}\varepsilon = 0.5\ E \tag{45}$$

and

$$^{2}\varepsilon = 0.75\ V\ . \tag{46}$$

Thus, the first three edge-connectivity indices for a fullerene are identical. In the case of buckminsterfullerene C_{60}: $^{0}\varepsilon = {}^{1}\varepsilon = {}^{2}\varepsilon = 45$.

CONCLUDING REMARKS

In recent years there was a considerable interest to compute topological indices of fullerenes.[10–14] These indices have been used for deriving structure-property relationships with the aim to predict various physicochemical properties of fullerenes, *e.g.,* Ref. 12. Here we have shown that explicit formulae can be derived for computing two types of connectivity indices for annulenes and fullerenes. These formulae are based solely on the number of vertices or edges in these compounds. Presumably many other kinds of topological indices can be also given in a closed form for annulenes, fullerenes and other families of compounds with highly regular structures.

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REFERENCES

1. F. Harary, *Graph Theory*, second printing, Addison-Wesley, Reading, MA, 1971, p. 14.
2. N. Trinajstić, *Chemical Graph Theory*, second revised edition, CRC Press, Boca Raton, FL, 1992, pp. 13–14.
3. M. Randić, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.
4. L. B. Kier, L. H. Hall, W. J. Murray, and M. Randić, *J. Pharm. Sci.* **65** (1976) 1226–1230.
5. E. Estrada, *J. Chem. Inf. Comput. Sci.* **35** (1995) 31–33.
6. Ref. 2, pp. 11–12.
7. M. Kunz, *Coll. Czech. Chem. Commun.* **55** (1990) 630–633.
8. E. Estrada, *J. Chem. Inf. Comput. Sci.* **35** (1995) 1022–1025.
9. N. Trinajstić, M. Randić, D. J. Klein, D. Babić, and Z. Mihalić, *Croat. Chem. Acta* **68** (1995) 241–267.
10. N. Trinajstić, S. Nikolić, D. Babić, and Z. Mihalić, *Bull. Chem. Technol. Macedonia* **16** (1997) 43–51.
11. C. M. White, *J. Chem. Eng. Data* **31** (1986) 198–208.
12. R. S. Ruoff, *Chem. Phys. Lett.* **208** (1993) 256–258.
13. N. Trinajstić, S. Nikolić, and Z. Mihalić, *Bull. Chem. Technol. Macedonia* **13** (1994) 61–68.
14. A. T. Balaban, X. Liu, D. J. Klein, D. Babić, T. G. Schmalz, W. A. Seitz, and M. Randić, *J. Chem. Inf. Comput. Sci.* **35** (1995) 396–404.

SAŽETAK

Indeksi povezanosti regularnih grafova

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Dane su eksplicitne formule za računanje prvih triju indeksa povezanosti čvorova i bridova regularnih grafova. U slučaju 2-regularnih grafova, koji služe npr. za modeliranje anulena, formule za indeks povezanosti čvorova i indeks povezanosti bridova identične su, jer je u tim grafovima broj čvorova jednak broju bridova. Kod 3-regularnih grafova, koji služe npr. za modeliranje fullerena, podudaraju se indeks povezanosti čvorova nultog reda i indeks povezanosti drugog reda, a prva su tri indeksa povezanosti bridova identična.