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Graph cyclicity, excess conductance, and resistance deficit

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A new graph-theoretic cyclicity index $C(G)$ is defined, being motivated in terms of mathematical concepts from the theory of electrical networks. This "global bond excess conductance" index $C(G)$ then is investigated, with a number of theorems as well as some discussion and numerical investigation. It is found that $C(G)$ typically has less degeneracy than the standard cyclomatic number and has some intuitively appealing features.

KEY WORDS: index $C(G)$, degeneracy, cyclomatic

1. Introduction

Electrical circuits provide a natural realization of graphs, and indeed have been so recognized since Kirchoff's [1] foundational paper of 1847, where some fundamental graph theoretical theorems were enunciated. Not too long after this molecular structures also began being represented as graphs, e.g., by Brown [2] in 1864. As it happens the mathematical field of graph theory was only recognized as a separate field somewhat later, really only fully developed in the twentieth century, with the first book on graph theory being that of Koenig [3] in 1937, and a sort of general recognition for the field arises perhaps only with Harary's book [4] of 1969. Early on Sylvester [5] in 1878 imagined an intimate contact between this then embryonic mathematical field and chemistry – and indeed he then seems to have introduced the phrase "graph" (or "graphoid") for these mathematical constructs, perhaps drawing this term from the chemical literature where structural molecular formulas were sometimes described as "graphical representations" (of molecules). Later (in 1937) Polya's fundamental combinatorial enumerative results [6] were largely motivated for related chemical applications. Still the field of chemical graph theory really has significantly developed within chemistry only over the last few decades, with an early (1976) edited book [7] being Balaban's on *Chemical Applications of Graph Theory* and a more recent (1983) nice text [8] in this overall area being Trinajstićs *Chemical Graph Theory*. The mathematical formalization of electrical network theory seems to have occurred more gradually and earlier (e.g., with some

mathematical theory of circuits found in Maxwell's famous treatise [9] of around 1900), but with varying degrees of development in different editions. A fairly elegantly well developed treatment is that of Reed and Seshu [10] in 1961. Indeed in the area of electrical network theory a number of novel theorems have been developed, with reaction back on the mathematical field, as exemplified in the charming book [11] of 1984 by Snell and Doyle. Thence it may be imagined that there too should be some valuable theory from the field of electrical networks for chemical applications. Indeed, the relative lack of such applications may seem especially surprising of in view of the fact that Kirchoff's original paper was in a "chemistry" journal. Only recently does it seem that some such suggestions have been seriously attended to, as in [12,13].

Here it is proposed to seek to develop the concept of "cyclicity" as motivated from electrical network theory, with the idea that this may prove useful for chemical graph-theoretic applications, and perhaps also for mathematical graph theory. The matter of the characterization of "cyclicity" is an aspect of key importance in the study of molecular graphs, e.g., as discussed by Bonchev and co-workers [14,15]. And in mathematics the idea of cyclicity is intimately related to measures of connectivity or complexity, e.g., as discussed by Tutte [16].

There are different possible measures of "cyclicity" of a graph G. One simple such traditional fundamental measure is the *cyclomatic number* $\mu(\mathrm{G})$ of a graph G with $N(\mathrm{G})$ vertices, $e(\mathrm{G})$ edges, and $k(\mathrm{G})$ components, whence

$$\mu(\mathrm{G}) \equiv e(\mathrm{G}) - N(\mathrm{G}) - k(\mathrm{G}). \tag{1}$$

This invariant is standardly found in most graph-theory texts, such as that of Harary [4], where it is noted to count the number of edge deletions it takes to make a graph acyclic. And this invariant is of key chemical relevance as may be exemplified for a (classical non-radicaloid) hydrocarbon represented by a carbon skeleton identified to G, for then this index $\mu = \mu(\mathrm{G})$ is involved in the overall molecular formula $\mathrm{C}_N\mathrm{H}_{2N+2-2\mu}$, whence too μ is some sort of degree of "unsaturation". But evidently then all species of the same isomer class have the same cyclomatic number, so that there are many graphs which μ does not distinguish. E.g., all monocycloalkanes $\mathrm{C}_N\mathrm{H}_{2N}$ have the same value $\mu = 1$, regardless of the value of N (and regardless of any saturated acyclic side structures). At least in chemical behavior many of the properties of such large-cycle cycloalkanes should approach those of corresponding open-chain normal alkanes $\mathrm{C}_N\mathrm{H}_{2N+2}$. Intuitively one might sense this, at least if one is concerned with properties dependent on local structure – properties such as heat of formation per carbon or magnetic susceptibility per carbon, or index of refraction. Of course, there are other properties which are undoubtedly somewhat different, say as depend on overall molecular conformation, whence the mean spatial extent of a cycloalkane might be but a fraction of that for the correspondent open-chain alkane. Of the chemical studies [14,15,17] devoted to a study of "cyclicity", most consider various already available indices as potential correlates to "cyclicity". Here we start *de novo*, seeking to develop a cyclicity graph invariant from a fundamental graph-theoretic/electrical-network perspective.

2. New cyclicity measure

In fact, the relevance of cyclicity is deeply embedded in electrical network theory (with trees and the cyclomatic number already evident in Kirchoff's original work [1]). To develop this perspective imagine a molecular graph G (with H atoms deleted) to correspond to an electrical network with "unit resistors" on each edge. Then if opposite poles of a battery are connected to different pairs of vertices of the network, different currents flow. Indeed there will be different effective *resistances* Ω_{ij} between different vertex pairs i and j – or equivalently there will be different effective *conductances*

$$\sigma_{ij} \equiv 1/\Omega_{ij}. \tag{2}$$

It is simply a matter of tradition that resistances rather than conductances are used in expressing Ohm's law. A conductance may be viewed as a sort of efficacy of communication between two sites. Now it turns out (as is well known) that Ω_{ij} (and thence also σ_{ij}) attends to the presence of multiple pathways between vertices, and as such might also be imagined to be of relevance in chemistry, where particular multiple pathways of length 1 (i.e., multiple bonds) are always recognized to be extremely important, and even for larger cycles notably different properties can arise, e.g., as occurs for the 6-cycle of benzene to make it dramatically different than linear hexatriene. Distances d_{ij} are plausibly relevant to "particulate communication" (or interaction) between vertices i and j while the resistance distance Ω_{ij} is plausibly relevant to a diffuse wave-like (i.e., multi-path) communication.

The resistances Ω_{ij} (and hence also the conductances σ_{ij}) are sensitive to the cycle structure of a graph G. Indeed, there is a fundamental result:

Ordering theorem for Ω and d. For a connected graph G, Ω_{ij} equals the length d_{ij} of the shortest path between i and j iff there is a unique single path between i and j, while if there is more than one path (even of different lengths), then Ω_{ij} is strictly less than d_{ij}.

See, e.g., [12]. Thence the *resistance deficit* $d_{ij} - \Omega_{ij}$ or the *conductance excess* $\sigma_{ij} - 1/d_{ij}$ indicate in some manner the presence of cyclicity in the portion of the graph interconnecting i and j. In fact these quantities detect the presence of cycles in the region between i and j regardless of whether i and j are themselves in a cycle. To more directly detect the mutual occurrence of i and j in a cycle one may focus on i and j which are adjacent, whence $d_{ij} - \Omega_{ij}$ and $\sigma_{ij} - 1/d_{ij}$ give non-zero values only if i and j are both in a mutual cycle. Thence we propose a *global cyclicity index* C(G) for a general graph G as

$$C(\mathrm{G}) \equiv \sum_{i-j}^{\mathrm{G}} \left(\sigma_{ij} - d_{ij}^{-1}\right) \tag{3}$$

where the sum is over all edges of G. This index may be interpreted as a "total excess bond conductance". With attention to resistances rather than conductances, our discussion suggests another possibility for a global cyclicity index as

$$\mu_{\star}(\mathrm{G}) \equiv \sum_{i-j}^{\mathrm{G}} (d_{ij} - \Omega_{ij}) \tag{4}$$

which may be interpreted as a "total bond resistance deficit". A further consequence of a focus on adjacent pairs of vertices, is that these formulas remain unambiguous (and finite so long as G is finite) regardless of whether G is connected or not. Here we investigate some characteristics of these cyclicity indices, and most especially $C(\mathrm{G})$.

3. Useful background framework

Though we have motivated our cyclicity indices in physical terms (as a global excess bond conductance or as a global bond resistance deficit), these indices are intrinsic to the graph G – i.e., $\mu'(\mathrm{G})$ and $C(\mathrm{G})$ are graph invariants. This is made more explicitly manifest in terms of the *Laplacian* matrix $\mathbf{L}$ (given as the diagonal degree matrix minus the adjacency matrix of G). It may be seen that for a column vector $\boldsymbol{x}$ with elements x_i that

$$\boldsymbol{x}^{\dagger}\mathbf{L}\boldsymbol{x} = \sum_{i-j}^{\mathrm{G}}(x_i - x_j)^2 \tag{5}$$

where the sum is over edges of the graph G. From this relation $\mathbf{L}$ is seen to be non-negative definite, and it may also be seen that $\mathbf{L}$ must have exactly one (independent) 0-eigenvalue eigenvector for each component of G – namely, the vectors which are constant on a component and 0 elsewhere. Thus $\mathbf{L}$ has a generalized inverse $\mathbf{\Gamma}$ which is 0 on the 0-eigenvalue eigenspace $\mathcal{V}_0$ of $\mathbf{L}$, and is a true inverse to $\mathbf{L}$ on the orthogonal component $\mathcal{V}_{\neq 0}$ to this null space. Then it turns out that for a connected graph G, the resistances Ω_{ij} for i and j within the same component of G are given in terms of the elements of $\mathbf{\Gamma}$, thusly

$$\Omega_{ij} = \Gamma_{ii} - \Gamma_{ij} - \Gamma_{ji} + \Gamma_{jj}. \tag{6}$$

Such has long been known in electrical network theory, though the development usually is for the case where different non-zero resistors r_{ij} are associated to edges $\{i, j\}$ of G, and one studies a weighted Laplacian (with off-diagonal elements $L_{ij} = -1/r_{ij}$). See, e.g., [7] or for a more purely graph-theoretic formulation see, e.g., [12]. For connected G, there are also other characterizations of Ω_{ij}:

- combinatorially in terms of trees and bi-trees [18];
- probabilistically in terms of random walks on G [11];
- as an intrinsic graph metric on each graph G [12]; and
- as a long-wave-length weighted amplitude-difference of eigen-wave-functions [20] on G.

In fact these definitions extend to disconnected graphs so long as the vertices i and j considered are in the same component of G – one merely takes the Ω_{ij} (and σ_{ij}) values to be the same as that with the single component being the whole graph – and for i and j in different components one naturally takes $\sigma_{ij} = 0$. Moreover it may be mentioned

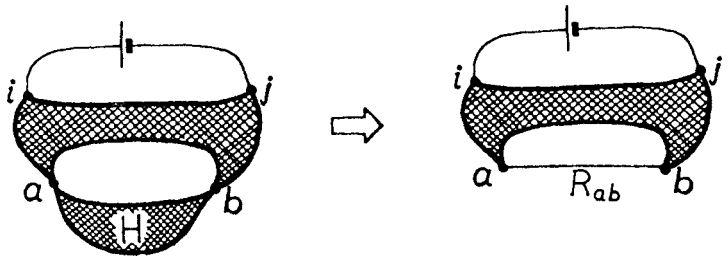


Figure 1. A depiction of the substitution rule, identifying an "equivalent circuit". Here the graph considered consists of the portion other than the top connection with a battery, which is introduced to identify the two vertices (i and j) between which the effective resistance is to be taken. The battery is reconnected to different pairs of vertices in considering different effective resistances Ω_{ij}, between these vertices. As mentioned in the text this effective resistance may be identified as a distance between i and j.

that Ω_{ij} provides [12] an intrinsic metric on a graph. It seems to us that especially the tree/bi-tree and probabilistic interpretations might also be neatly used to motivate our cyclicity indices.

In establishing our theorems for the global cyclicity index, we use a few well-known results for electrical networks. These are best stated if allowance is made for resistors of different values to be associated with different edges of a then weighted graph, whence in such a case the values of the resistors on the edges are appended as labels to the edges.

Substitution rule. Let a graph G have a connected subgraph H joined *via* only two of its vertices a and b to the rest of the graph, let any edge between a and b be included in H, let the effective resistance in H between a and b be R_{ab}, and let i and j be two vertices of G such that neither i nor j is a vertex in H other than a or b. Then the effective resistance Ω_{ij} is equal to that between the graph G_H with all of H deleted from G excepting vertices a and b which are connected with a new edge of weight R_{ab}.

This rule might be depicted as in figure 1. The utility of this rule (or theorem) is made manifest if one has effective resistances for a few elementary subgraphs, such as a cycle and a chain.

Series rule. Let a and b be the two terminal vertices of an edge-weighted chain graph. Then the resistance R_{ab} is the sum of the edge weights.

Parallel rule. Let a and b be two vertices of an edge-weighted subgraphs, and let R_1 and R_2 be the sums of the edge weights along the two paths between a and b. Then the inverse of the resistance between a and b is the sum of the inverses of R_1 and R_2.

In fact these three "rules" (which are in fact theorems) are found not only in electrical circuit theory texts, but usually are developed in introductory physics texts. Thence millions of people are aware of these rules, though not all effective resistances for all circuits can be so obtained (using just series and parallel substitutions). Also related to the substitution rule there is a related result:

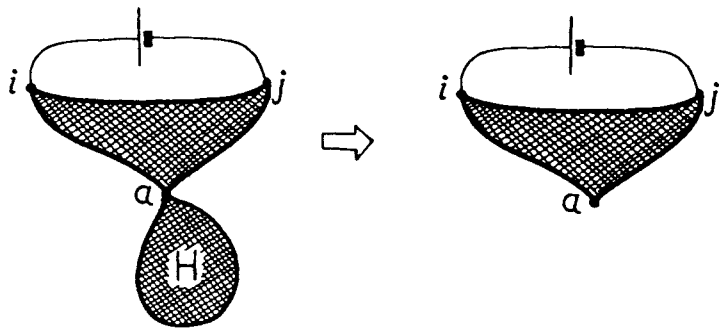


Figure 2. A depiction of the elimination rule, identifying "equivalent circuts".

Elimination rule. Let H be a subgraph of G connected to the rest of G via only a single vertex a, as in the substitution theorem, and let i and j be two vertices in H. Then the effective resistance Ω_{ij} between i and j in G is the same as that Ω'_{ij} between i and j in H.

This may be depicted as in figure 2. In fact this theorem really is only physically plausible. Basically if a battery is connected between vertices i and j of the subgraph H of this theorem, then there can be no flow of current outside the subgraph H for it would need to flow through vertex a to or from the remaining part of the graph where there is no source or sink. In fact, in the physical context, e.g., of the development of section 2 of [12], this in essence constitutes a proof. With these few standard sorts of "rules" in hand the bulk of the results of the next section turn out to be fairly readily establishable.

4. Statement and discussion of theorems

Our theorems, corollaries, and lemmas are stated in this section along with a discussion of their meaning and interpretation. The proofs are given in the next section following.

As a first point the formulas for the two indices C and $\mu_\star$ may be recast in terms of matrices $\mathbf{\Omega}$ and $\boldsymbol{\sigma}$ with respective elements Ω_{ij} and σ_{ij}. Then:

Theorem A. If G is a graph with e(G) edges and an adjacency matrix $\mathbf{A}$, then

$$C(\mathrm{G}) = \mathrm{tr}\{\boldsymbol{\sigma}\mathbf{A}\} - e(\mathrm{G}) \quad \text{and} \quad \mu_\star(\mathrm{G}) = e(\mathrm{G}) - \mathrm{tr}\{\mathbf{\Omega}\mathbf{A}\}$$

where tr denotes the trace operation.

That is, these indices are given in terms of matrix invariants And as a second point we may consider the index $\mu_\star$, which though not our prime focus, does clearly turn out to be a cyclicity index, because:

Theorem B. For any graph G, $\mu_\star(\mathrm{G}) = \mu(\mathrm{G})$.

That is, $\mu_\star$ provides naught but a reinterpreted form (as a global bond resistance deficit) for the standard cyclomatic number.

Of prime focus here is the cyclicity index C. Support for C being a cyclicity index is attained from the close correspondence and favorable result (of theorem B) for $\mu_\star$. In addition we have:

Theorem C. For an arbitrary graph G, $C(\mathrm{G}) \geqslant 0$ and $\mu(\mathrm{G}) \geqslant 0$, with equality for exactly the same G – that is, $C(\mathrm{G}) = 0$ iff $\mu(\mathrm{G}) = 0$.

Both $C(\mathrm{G})$ and $\mu(\mathrm{G})$ turn out to have identical values for acyclic graphs, though even in such a circumstance the new index $C(\mathrm{G})$ has a somewhat different interpretation (as a global excess bond resistance). Further similarity between C and μ may be adduced if we define a *kernal* G$\downarrow$ of a graph G to be a new graph obtained from G by repetition of certain "deletion" transformations:

- degree-0 sites are deleted; and
- edges which if deleted would leave two new disconnected fragments, are deleted;
- a site as i which if deleted would leave two new disconnected fragments H and K, is used to construct two graphs: H_+ isomorphic to that induced from the vertices of H along with i, and K_+ isomorphic to that induced from the vertices of K along with i.

Such a kernal G$\downarrow$ contains no degree-1 vertices nor what are frequently termed "isthmuses" or "bridges". An illustrative example is provided in figure 3. For a tree G it turns out that G$\downarrow$ is the empty graph (in which case $C(\mathrm{G}) = 0$). The third type of transformation here gives two subgraphs which might be viewed to share a common vertex i, but we view one of the two new graphs H_+ and K_+ rather to involve a "copy" of the common vertex so that H_+ and K_+ are disjoint. Now we have:

Theorem D. For any graph G, $\mu(G) = \mu(\mathrm{G}\downarrow)$ and $C(\mathrm{G}) = C(\mathrm{G}\downarrow)$.

Still C and μ seem similar. For some cases similarity short of identity (between the values of C and μ) applies:

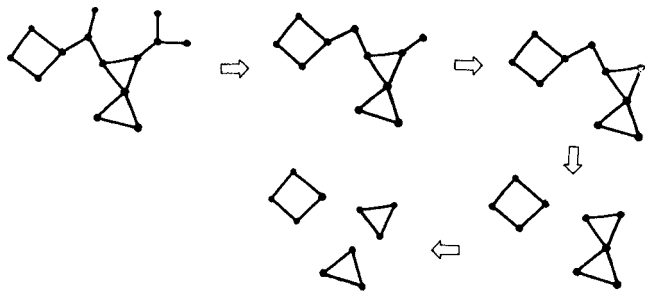


Figure 3. Example of transformations leading from a graph G to its kernal G$\downarrow$.

Theorem E. For any connected graph G with $\mu(\mathrm{G}) = 1$, G has a single cycle of some size n ($\geqslant 3$) and $C(\mathrm{G}) = n/(n-1)$.

Here for G with $\mu(\mathrm{G}) = 1$ this theorem implies that $C(\mathrm{G})$ approaches $\mu(\mathrm{G})$ as the size of the single cycle becomes very large. At the same time $C(\mathrm{G})$ seems to be less degenerate than $\mu(\mathrm{G})$, and to conform to our introductory intuitive suspicion that of the simple N-vertex single-cycle graphs c_N, those with larger N should be less cyclic. Further one sees that though $\mu(\mathrm{G})$ is invariant under homeomorphism transformations (where "contractions" may take place at degree-2 sites), $C(\mathrm{G})$ is not generally invariant under such transformations (for otherwise all cycles c_N would have the same value for $C(\mathrm{c}_N)$ for all $N \geqslant 3$). We further have:

Theorem F. Let G be a graph G with a kernal G$\downarrow$ consisting of two disjoint graphs H and K. Then $\mu(\mathrm{G}) = \mu(\mathrm{H}) + \mu(\mathrm{K})$ and $C(\mathrm{G}) = C(\mathrm{H}) + C(\mathrm{K})$.

This again emphasizes a similarity between μ and C, and in particular for any disconnected graph both C and μ are the sums of the corresponding values for the different components. This theorem also leads to:

Corollary G. Let G be a connected graph with a kernal G$\downarrow$ which is a set of n disjoint cycles. Then $\mu(\mathrm{G}) = n$ and

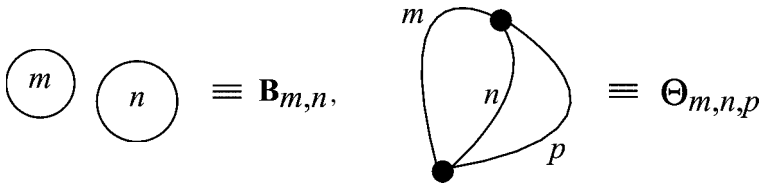
$$C(\mathrm{G}) = \sum_{q=1}^{n} \frac{n_q}{n_q - 1}$$

with n_q the size of the qth cycle of G$\downarrow$.

Evidently now we can see that sometimes even when μ is not degenerate, our cyclicity index C can turn out to be degenerate: e.g., if G$\downarrow$ consists of six disjoint 3-cycles and G$'\downarrow$ consists of seven disjoint 8-cycles, then $C(\mathrm{G}) = 8 = C(\mathrm{G}')$. Note too that the example need not be confined to disjoint cycles, but may involve connected graphs G and G$'$ with the indicated disconnected kernals. Still from theorem E and corollary G it seems that the more typical case is that C is less degenerate than μ.

In-as-much-as graphs with cyclomatic numbers $\mu(\mathrm{G}) = 0$ and 1 have now been quite fully treated one might next focus on those with $\mu(\mathrm{G}) = 2$. Thence we note that:

Lemma H. If G is a connected graph with $\mu(\mathrm{G}) = 2$, then G is planar and has a kernal G$\downarrow$ of one of the two forms



where m, n, p identify lengths of indicated cycles in the first form and of paths in the second form.

Evidently the index for such a graph with a kernal of the first form is covered by corollary G, while for one with a kernal of the second form, we have:

Theorem I. If G is an N-vertex connected graph with $\mu(\mathrm{G}) = 2$ and a kernal $\mathrm{G} = \Theta_{m,n,p}$, then

$$C(\mathrm{G}) = \frac{m(p+n)}{S-p-n} + \frac{n(p+m)}{S-m-p} + \frac{p(m+n)}{S-n-m}$$

where $S \equiv mn + np + pm$.

One might imagine seeking to go on explicitly to the next higher cyclomatic number:

Observation J. If G is a connected graph with $\mu(\mathrm{G}) = 3$, then G is planar and there are but five possible types of kernals G$\downarrow$, of one of the forms in figure 4.

The index C for such graphs with a kernal of the first two (disconnected) forms are covered by the results E, F, and I previously, and presumably formulas such as given in theorem I could be developed for the remaining three forms.

In addition to the transformations which reduce a graph to its kernal, there are also some other transformations which leave $C(\mathrm{G})$ invariant:

Observation K. If a transformation of a graph G is made to G$'$ with one edge e moved about in a cycle so that whatever cycles e is in, e retains membership therein, then $C(\mathrm{G}') = C(\mathrm{G})$.

A specialization of this result might be made, to simplified circumstances of common chemical relevance:

Theorem L. Let G be graph with a cycle c which if deleted leaves disconnected components, $\mathrm{H}_1, \mathrm{H}_2, \ldots, \mathrm{H}_m$ such that each component connects to c either at a single site or at a single edge. Let H_a^+ be that graph induced from H_a and whatever vertices in c to which H_a connects. Then any edge e of c may be moved about in c along with whatever H_a^+ this edge might be in so as to obtain another graph G$'$ with $C(\mathrm{G}') = C(\mathrm{G})$. If a fragment H_b^+ shares only a single site i with c and only a single site with e, then whether or not H_b^+ is moved with e does not affect the value of the cyclicity index C.

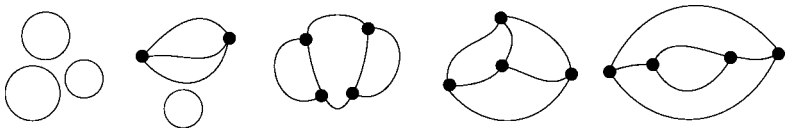


Figure 4. The five general forms for kernals G$\downarrow$ of graphs G with $\mu(\mathrm{G}) = 2$.

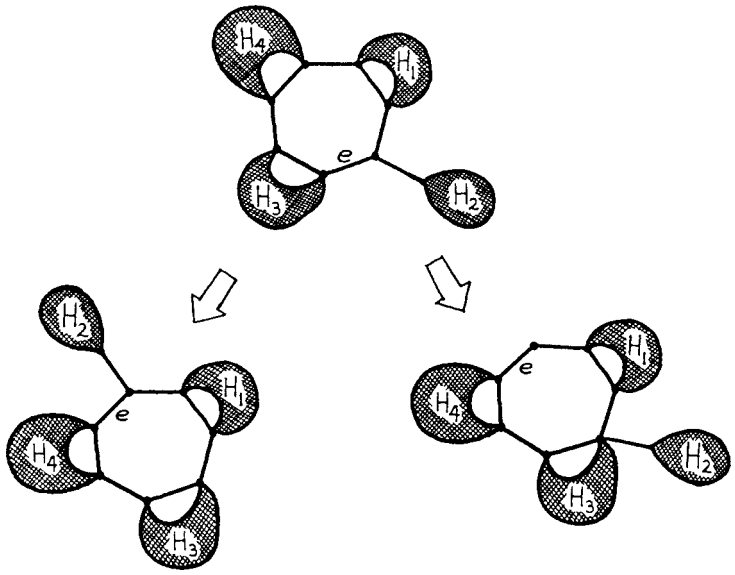
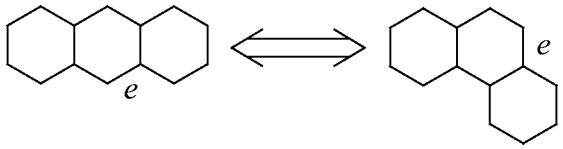


Figure 5. An example of the size-conserving C-fixed transformation of theorem L.

The circumstance is depicted in figure 5. A chemically relevant example of such a transformation of this type is that which interchanges anthracene and phenanthrene graphs:



That is, C identifies these two graphs to be of the same cyclicity $C(\mathrm{G}) = 116/31 \approx 3.74194$. Indeed because benzenoids are of much interest, we might direct attention to the case of a *phenacenic* chain of fused benzene rings, the non-terminal rings of which may be fused in either of the two patterns of the central rings of anthracene or of phenanthrene. Then:

Corollary M. Every phenacenic chain with the same number h of hexagons has exactly the same cyclicity index, C_h.

That is, the $\sim 3^h$ such isomeric phenacenic chains of h hexagonal rings exhibit degeneracy. Indeed we might list the first few values:

$$\begin{array}{llll} C_1 = 6/5, & C_2 = 358/145 \approx 2.4690, & C_3 \approx 3.7419, & C_4 \approx 5.0151, \\ C_5 \approx 6.2883, & C_6 \approx 7.5614, & C_7 \approx 8.8346, & C_8 \approx 10.10775, \\ C_9 \approx 11.3809, & C_{10} \approx 12.6541, & C_{11} \approx 13.9272, & C_{12} \approx 15.2004, \\ C_{13} \approx 16.4736, & C_{14} \approx 17.7467, & C_{15} \approx 19.0199, & \ldots \end{array} \tag{7}$$

Moreover, for this sequence, a near linear relation is perceived for the values, so that they are closely approximated by

$$C_h \approx A \cdot h - B, \quad A \approx 1.273162 \text{ and } B \approx -0.077553, \tag{8}$$

as obtained by least squares fitting the numerical data for $h = 3 \rightarrow 60$. This result is quite accurate, with r being 1 to less than 10^{-6}, a standard deviation $s \cong 10^{-6}$.

We surmise that many different homologous sequences of molecular species should exhibit similar regular asymptotic behaviors. If there is a single bond interconnecting adjacent monomer units, then the linearity in the number of such units is exact.

Finally, some results are available for suitably regular graphs (even of higher cyclicities):

Theorem N. For a connected N-vertex d-regular edge-transitive graph G,

$$C(\mathrm{G}) = \frac{N}{N-1}\left(1 + N\frac{d-2}{2}\right) = \mu(\mathrm{G}) + \frac{N}{N-1}\frac{d}{2}.$$

In particular, this applies to the graphs of the regular polyhedra, such as have been of some interest, even in connection [13,20] with resistance distances. Thence we may note:

Corollary O. For the graphs of the regular polyhedra

$$C(\mathrm{K}_4) = 4, \qquad C(\mathrm{Q}_3) = \frac{40}{7} \approx 5.71, \qquad C(\mathrm{O}_3) = \frac{42}{5} = 8.4,$$

$$C(\mathrm{D}) = \frac{220}{19} \approx 11.58, \qquad C(\mathrm{I}) = \frac{228}{11} \approx 20.73$$

where K_4, Q_3, O_3, D, and I respectively denote the graphs of the tetrahedron, cube, octahedron, dodecahedron, and icosahedron.

For comparison the cyclomatic numbers of the regular polyhedral graphs may be noted:

$$\mu(\mathrm{K}_4) = 3, \quad \mu(\mathrm{Q}_3) = 5, \quad \mu(\mathrm{O}_3) = 7, \quad \mu(\mathrm{D}) = 11, \quad \mu(\mathrm{I}) = 19. \tag{9}$$

Evidently the values are in the same order. More generally, theorem N applies to the graphs of regular polytopes, and other regular graphs (such as the complete bipartite graphs $\mathrm{K}_{n,n}$ and the "Peterson" graph, such as appears in the logo on the present journal).

5. Proofs

First, in the definition of $\mu_\star$ and C one may introduce the adjacency matrix **A** which has elements A_{ij} which are 0 except when i and j are adjacent in the graph G. Then with e the number of edges in G,

$$\mu_\star(\mathrm{G}) = e - \left(\sum_{i,j} \Omega_{ij} A_{ji}\right) \quad \text{and} \quad C(\mathrm{G}) = \left(\sum_{i,j} \sigma_{ij} A_{ji}\right) - e \tag{10}$$

where now the sums are over all pairs of vertices. Thence theorem A is obtained.

The proof of theorem B builds upon the first of the expressions above. Since $\Omega_{ii} = 0$, one may add in a diagonal matrix such as that with the degree d_i of the ith site at the ith position along the diagonal, to obtain

$$\mu(\mathrm{G}) = e + \sum_{i,j} \Omega_{ij} \frac{d_j \delta_{ji} - A_{ji}}{2} = e + \sum_{i,j} \Omega_{ij} L_{ji} = e + \sum_{i,j} \frac{(\Gamma_{ii} - 2\Gamma_{ij} + \Gamma_{jj}) L_{ji}}{2}. \tag{11}$$

Now noting that the column vector $\boldsymbol{\varphi}$ with all components $\varphi_i = 1$ is an eignevector to $\mathbf{L}$, one sees that (single-index) sums such as $\sum_j \Gamma_{jj} L_{ji} = \sum_j \Gamma_{jj} (\mathbf{L}\boldsymbol{\varphi})_i = 0$, while the sum $\Sigma_j \Gamma_{ij} L_{ji}$ must give the (i,i)th element of the projection $\mathbf{P}$ onto the non-null subspace of $\mathbf{L}$, and this we have already noted (near equation (5)) is $(N-1)$-dimensional for an N-vertex connected graph. Thus for such a graph

$$\mu(\mathrm{G}) = e - \sum_{i,j} \Gamma_{ij} L_{ji} = e - \sum_i P_{ii} = e - (N-1). \tag{12}$$

Now for a graph with a general number k of components, the whole argument proceeds similarly, except that the null space of $\mathbf{L}$ (and thence too of $\mathbf{\Gamma}$) is k dimensional, as may be seen from equation (5). Thence the projector $\mathbf{P} = \mathbf{\Gamma L}$ has a non-null space ($\mathcal{V}_{\neq 0}$) of dimension $N - k$, and

$$\mu(\mathrm{G}) = e - N + k \tag{13}$$

thereby establishing theorem B. In fact, the connected graph case is an immediate consequence of a known theorem that for such graphs the sum over nearest-neighbor effective resistances gives $N - 1$. This was originally proved by Foster [21], and independently rediscovered [12,22] a couple of times.

For theorem C the obvious (and well-known) fact that $\mu(\mathrm{G}) \geqslant 0$ is here stated to draw the parallel to the new invariant $C(\mathrm{G})$. For the more substantive part of this theorem we may make use a result noted in the introduction, that for a connected graph $\Omega_{ij} \leqslant d_{ij}$ with equality iff there is but one path between vertices i and j. (See, e.g., [12], but also it may be worked out using the elimination rule and the series rule of the background section.) Thence, for neighbor pair $\{i, j\}$ of sites we have $\Omega_{ij} - d_{ij} \geqslant 0$ with equality iff i and j are in a common cycle G, so that for a sum of $\Omega_{ij} - d_{ij}$ over all neighbor pairs, one obtains equality to 0 iff no two neighbor sites occur in a cycle. That is, this sum is $\geqslant 0$ with equality iff G is acyclic (as occurs iff $\mu(\mathrm{G}) = 0$), and theorem C is established.

Next consider a connected graph G with an edge $\{i, j\}$ between vertices i and j such that this edge occurs in no cycle of G, and let a new graph G_- be that with this edge deleted. Now from the argument for theorem C we see that $\Omega_{ij} = 1$ in G, so that $\Omega_{ij} - 1 = 0$, and makes no contribution to $C(\mathrm{G})$, and of course there is no Ω_{ij} contribution in $C(\mathrm{G}')$ either. Further the edge $\{i, j\}$ of G may by the substitution theorem be deleted in computing Ω_{e} for any other edge e in G. Thus $C(\mathrm{G})$ has no net effect from the edge $\{i, j\}$ at all, so that $C(\mathrm{G}_-) = C(\mathrm{G})$, and iteration of such deletions yields theorem D.

If $\mu(\mathrm{G}) = 1$, then G is one edge short of being acyclic and thus contains a single cycle with possibly some acyclic appendages or also possibly some additional acyclic components. Then G$\downarrow$ is a single cycle of the size n, and the parallel rule implies that for any edge e of G$\downarrow$ one has $\Omega_{\mathrm{e}} = \{1 + 1/(n-1)\}^{-1} = (n-1)/n$. Using this result in the defining formula for C, then gives $C(\mathrm{G}\downarrow) = n(\Omega_{\mathrm{e}} - 1\} = n/(n-1)$, and by theorem D the index $C(\mathrm{G})$ (as well as theorem E) is obtained.

For theorem F we note that if G$\downarrow$ = H $\cup$ K, then by theorem C we have $\mu(\mathrm{G}) = \mu(\mathrm{H} \cup \mathrm{K})$ and $C(\mathrm{G}) = C(\mathrm{H} \cup \mathrm{K})$. But the definitions of μ and C directly imply that these indices for a disjoint union of two graphs as H and K are given as the sums of the corresponding indices for H and K, so that theorem F is established.

Corollary G follows directly from theorems E and F.

For a graph with $\mu(2)$ there must be two cycles, which if they share no edge then give G$\downarrow$ as two disjoint cycles (say of sizes m and n). If on the other hand the two cycles (say of sizes m and p) share some positive number n of edges, then these edges must be contiguous, for otherwise there would be additional cycles, so that it is seen that G$\downarrow$ is a "theta" graph as in the theorem H, which is now established.

For theorem I we consider a typical edge e in one path of $\Theta_{m,n,p}$. If e is in the path of length m, then in computing its effective resistance Ω_m, we use the substitution rule to replace the two other now parallel paths (of lengths n and p) by a single edge of weight $R_m = \{n^{-1} + p^{-1}\}^{-1}$. Then e appears in a single (weighted) cycle (with m edges of weight 1 and one edge of weight R_m), so that $1/\Omega_m$ is the sum of the inverses of the net weights for the two paths between the terminuses of e. That is,

$$\Omega_m = \left\{1^{-1} + (m - 1 + R_m)^{-1}\right\}^{-1} = \left\{1 + \frac{p+n}{S-p-n}\right\}^{-1} \tag{14}$$

where $S \equiv mn + np + pm$. Similar formulas apply for effective resistances (Ω_n and Ω_p) for adjacent vertices in the other paths (the various lengths m, n, p just being permuted about. But with m, n, and p being edges with respective effective resistances of Ω_m, Ω_n, and Ω_p we have

$$C(\Theta_{m,n,p}) = m(\Omega_{\mathrm{m}} - 1) + n(\Omega_n - 1) + p(\Omega_p - 1) \tag{15}$$

which (with the use of equation (14)) reduces to the formula of theorem I.

A proof of observation J presumably proceeds in somewhat the same manner as that for lemma H, but is more involved, and is not gone into here.

Also a proof of observation K is not sought, but rather one for the theorem L. For the graph G with cycle c as in the hypothesis consider the value of $\Omega_{i,j}$ for an adjacent pair of vertices i and j of c but with this edge $\{i, j\}$ not in any H_a^+, in which case $\Omega_{i,j}$ is given as the resistance between the adjacent i and j in a (weighted) single cycle graph c_W with each of the H_a^+ fragments of G replaced by a suitable weight R_a as described in the substitution rule. But this resistance $\Omega_{i,j}$ does not depend on the orders of the edges in c_W. Next consider a different pair of adjacent vertices i and j now in one of the H_a^+, whence all of the H_b^+ for $b \neq a$ may be replaced by the R_b-weighted edges in a weighted c'_W, and the various edges may again be permuted about without changing $\Omega_{i,j}$. Thence

no effective resistance for any nearest-neighbor pair depends on the order of the edges in c, and the theorem is established. Corollary M follows quite directly.

To establish theorem N we again use the theorem mentioned in the second paragraph of this section. For an N-vertex connected graph G this identifies $N-1$ to the sum over all nearest-neighbor effective resistances. But for an edge transitive graph each effective resistance for an edge must take the same value Ω_1, while the number of edges of a d-regular graph is $Nd/2$, so that we have $\Omega_1 = 2(N-1)/dN$. Thence the formula for $C(\mathrm{G})$ as in theorem M results.

Corollary O is a direct consequence of theorem N.

6. Further discussion and overview

From our investigation mostly via a suite of theorematic results, it seems our global cyclicity index $C(\mathrm{G})$ for a graph G behaves somewhat like the traditional cyclomatic number $\mu(\mathrm{G})$. However, $C(\mathrm{G})$ is typically less degenerate and further conforms to some additional intuitively appealing features discussed in the introduction. This index $C(\mathrm{G})$ is a global excess bond conductance, whereas the alternative cyclicity index $\mu_\star(\mathrm{G})$ is a global bond resistance deficit and behaves identically to the traditional cyclomatic number $\mu(\mathrm{G})$.

The work of Bonchev and co-workers has considered other indices as indicators of cyclicity. In particular, the Wiener number

$$W(\mathrm{G}) \equiv \sum_{i<j} d_{ij} \tag{16}$$

was originally so considered [14], with its value for "similar" systems increasing with increasing cyclicity. Later [15] the resistance-distance analog (there called the "Kirchoff number")

$$W'(\mathrm{G}) \equiv \sum_{i<j} \Omega_{ij} \tag{17}$$

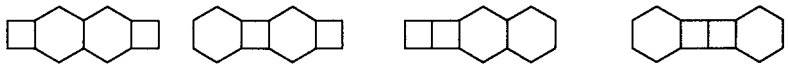
was similarly considered, and also noted was the so-called "Harary number"

$$H(\mathrm{G}) \equiv \sum_{i<j} \frac{1}{d_{ij}} \tag{18}$$

considered as a possibility to distinguish certain G with the same value of $W(\mathrm{G})$. It might seem natural also to consider the resistance-distance analog

$$H'(\mathrm{G}) \equiv \sum_{i<j} \sigma_{ij}. \tag{19}$$

One of the there-perceived advantages for $W'(\mathrm{G})$ over $W(\mathrm{G})$ was that $W'(\mathrm{G})$ typically seems to be less degenerate. For instance, for the four graphs of figure 6 the Wiener indices are all the same (with value 277) while $W'(\mathrm{G})$ was found to distinguish them. The corresponding values for our cyclicity index $C(\mathrm{G})$ are also found to be non-degenerate,



5.371	5.422	5.452	5.504
23.870	24.187	24.073	24.460
121.131	120.907	120.583	120.373
$4^2,6^3,8^2,10^2,14^1$	$4^2,6^3,8^1,10^2,12^1,14^1$	$4^2,6^2,8^3,10^1,12^1,14^1$	$4^2,6^2,8^2,10^1,12^2,14^1$

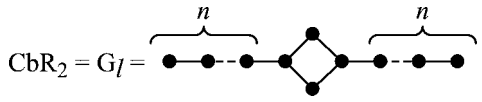
Figure 6. The four catacondensed linear-chain graphs G comprised of two 4-membered rings and two 6-membered rings. All four have the same Wiener index (=277), the same "Harary" index (≈41.45), and the same cyclomatic number (=4). The values for $C(\mathrm{G})$, $H'(\mathrm{G}) - H(\mathrm{G})$, and $W(\mathrm{G}) - W'(\mathrm{G})$ are listed below each graph, and finally the cycle distribution is listed for each.

as also indicated in the figure, and indeed one sees that the two indices ($C(\mathrm{G})$ and $W'(\mathrm{G})$) order these graphs similarly. Also noted in figure 6 are values for a couple other indices (to be discussed in the next paragraph) along with the distribution of cycles for each graph, with a term n^m indicating that there are m cycles of size n. Evidently the ordering of these graphs by $C(\mathrm{G})$ increases with the shift of the distribution of cycles to smaller cycles (such as we have already considered more cyclic). We emphasize that either $W(\mathrm{G})$ or $W'(\mathrm{G})$ can be only qualitative indicators of cyclicity, e.g., since they give non-zero results for trees.

A further aspect of our argument in the introduction for the definition of $C(\mathrm{G})$ and $\mu_\star(\mathrm{G})$ concerned the summation only over edges of G, rather than over all pairs of vertices. The alternative of the summation over all vertices, would bring to the fore the difference indices

$$\sum_{i<j}(d_{ij} - \Omega_{ij}) = W(\mathrm{G}) - W'(\mathrm{G}) \quad \text{and} \quad \sum_{i<j}(\sigma_{ij} - d_{ij}^{-1}) = H'(\mathrm{G}) - H(\mathrm{G}). \tag{20}$$

Our argument in the introduction was that for general pairs i and j the differences $\sigma_{ij} - d_{ij}^{-1}$ and $d_{ij} - \Omega_{ij}$ can be non-zero even when i and j are not in a mutual cycle. This may be illustrated for the 1,3-dialkyl-cyclobutane graphs



where R represents an alkyl chain R of some length n. Then

$$C(\mathrm{G}_n) = \frac{4}{3} \quad \text{and} \quad \mu_\star(\mathrm{G}_n) = \mu(\mathrm{G}_n) = 1, \qquad \text{for all } n \geqslant 0 \tag{21}$$

while

$$\sum_{i<j}\left(\sigma_{ij} - d_{ij}^{-1}\right) \approx 2.33, 3.04, 3.46, 3.76, 3.99, 4.17, 4.33, \ldots$$

$$\sum_{i<j}(d_{ij} - \Omega_{ij}) = 3, 7, 13, 21, 31, 43, 57, 73, 91, 111, \ldots \tag{22}$$

for $n = 0, 1, 2, 3, 4, 5, 6, \ldots$.

Evidently, as n increases these species lead to ever increasing values for these indices involving sums over all pairs of vertices, and in the case of resistance deficits even leads to a divergent sequence, although we intuit that the cyclicity of these species (with a ring of fixed size which is an ever smaller fraction of the whole) should not increase. That is, these full vertex-pair sum indices do not seem to us to fulfill the conditions of a good cyclicity index. The summands in our definitions for $C(\mathrm{G})$ and $\mu_\star(\mathrm{G})$ give non-zero contributions iff the two adjacent vertices labelling the summand are within a common cycle, and then the contribution is positive (as noted in our "Ordering theorem for Ω and d").

Other interesting graph invariants of potential chemical relevance might be expected. One might define a mean bond excess conductance invariant as $C(\mathrm{G})/e(\mathrm{G})$, as some sort of mean cyclicity contribution per bond. And other cyclicity indices paying attention to conductance excesses (or resistance deficits) for pairs of vertices farther apart than neighbors might be of value to investigate. The further fact that Ω_{ij} is [12] an intrinsic graph metric further supports the fundamentality of these electric-network-based ideas. With this in mind it has been suggested [23] that this metric could appropriately termed the "electric metric". But we still prefer the earlier name of "resistance distance", in part because the electrical interpretation is but one possibility (as noted in our discussion at and following equation (6)).

Further it may be noted that there are a number of invariants which have been suggested [24–27] based on matrix inversion problems related to that of computing the generalized inverse $\mathbf{\Gamma}$ somewhat similar to what is done for applications utilizing electrical-network ideas. Indeed Gollender et al. [24] are motivated by electrical network theory and speak of a network of "potentials" on the sites, but instead of $\mathbf{L}$ and its generalized inverse $\mathbf{\Gamma}$, they use $\mathbf{I} + \mathbf{L}$ (with $\mathbf{I}$ the identity matrix) and its true inverse $(\mathbf{I} + \mathbf{L})^{-1}$, whence with the ensuant manipulations it seems that different sorts of invariants (and "potentials" other than electrical potentials) arise. More generally, such manipulations merge into the theory of the Laplacian matrix, which may be perceived as of wider significance than electrical network theory. Thence in other contexts $\mathbf{L}$ has been somewhat used in chemistry, as in [28–31], and fairly intensively treated in mathematical graph theory – e.g., as reviewed in [32–34]. Notably Fiedler's Laplacian-based "geometric" results [35] have a neat interpretation (and extension) in terms of our metric ideas [19].

Overall it seems that we have an interesting new graph invariant $C(\mathrm{G})$, a global excess bond conductance which is a cyclicity measure. A related global bond resistance deficit $\mu_\star(\mathrm{G})$ is found to be the ordinary cyclomatic number. General support is thus garnered for the general contention [12,13,15,19,20,31] that resistance distance and related electrical-network ideas may have wide (chemical) graph-theoretic application. The novelty of this general idea is attested to by the fact that the associated resistance-distance metric (Ω) is not found in the comprehensive book [36] of Buckley and Harary on graph distances. Thence it is hoped that the present and earlier work on this metric and related ideas should prove of interest not only for chemists but also graph theoreticians, such as Professor Frank Harary, to whom we dedicate this article on the occasion of his 80th anniversary of his birthday.

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