# RECIPROCAL SPANNING-TREE DENSITY: A NEW INDEX FOR CHARACTERISING THE INTRICACY OF A (POLY)CYCLIC MOLECULAR-GRAPH*

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**Abstract.** Two quantities are defined, called *spanning-tree density* and *reciprocal spanning-tree density*, and they are then used to discuss the structural intricacy of a number of graphs of chemical interest.

## INTRODUCTION

In this work, we introduce and evaluate a concept that leads to the definition of two new indices that we shall call '*spanning-tree density*' and '*reciprocal spanning-tree density*', in an attempt to quantify how structurally 'complicated' a polycyclic molecular-graph actually is — a hitherto somewhat qualitative attribute that we shall henceforth refer to as the *intricacy* of such a graph. This latter has been dubbed by several authors [1-6] (including one of us [3]) the *complexity* of the molecular graph in question. This term is, however, liable to give rise to misunderstandings, for mathematicians (*e.g.*, refs. 7–11, and pp. 38, 50 and 225 of ref. 12) and chaos-theorists (*e.g.*, ref. 13) reserve the word 'complexity' simply to denote the number of spanning trees in a graph; the two of us have (independently) used 'complexity' with this connotation on several occasions [14–23] as a well-defined, strictly quantitative, numerical property of a molecular graph.

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*Dedicated to Professor Horst Sachs on the occasion of his 75th birthday.

'Complexity' as more generally used by chemical graph-theorists, on the other hand, is a somewhat vague and avowedly qualitative term that does, however, frequently run parallel with other intuitive, semi-quantitative chemical-terms (such as aromaticity, branching, cyclicity *etc.*) that are in daily use by chemists. Nevertheless, many attempts to define and measure 'complexity' have been published, and a book on this subject is soon to appear [24].

The first authors who suggested simply using the number of spanning trees (what they referred to as *maximal trees*) as a measure of what we are here calling the intricacy of a graph were Bonchev *et al.* [25,26], some twenty years ago. Their criterion was straightforward: the greater the number of spanning trees, the more 'complex' the structure. Recall that a spanning tree of a graph $G$ is a connected, acyclic sub-graph that comprises all the vertices of $G$ (see p. 46 of ref. 27 and pp. 12 and 63 of ref. 28). Since the spanning tree of a graph that contains no cycles is, identically, just the graph itself, it is obviously feasible to use the number of spanning trees as a measure of graph intricacy in the case of (poly)cyclic structures *only*; the same is true for our two new indices, *spanning-tree density* and *reciprocal spanning-tree density*, both defined in the next section.

## SPANNING-TREE DENSITY AND RECIPROCAL SPANNING-TREE DENSITY

In a simple graph, $G$ (*i.e.*, one without multiple edges), with $v$ vertices and $e$ edges, any spanning tree must contain precisely $(v-1)$ edges. The number of ways of choosing any $(v-1)$ edges from the $e$ available edges is ${}^{e}C_{(v-1)}$. Now, of course, not every such set of $(v-1)$ edges so selected will constitute a spanning tree of $G$ when the remaining edges in $G$ are deleted. If $t(G)$ represents the number of spanning trees of $G$, then we *define* the *Spanning-Tree Density* of $G$ (denoted by the symbol STD($G$)) as the *ratio*

$$(t(G)) / ({}^{e}C_{(v-1)}).$$

It may be thought of as representing the *probability* that if *any* set of $(v-1)$ edges in $G$ is selected, and the other $(e-v+1)$ edges in $G$ are deleted, the resulting entity is a spanning tree. In order to be able to deal with numbers that are greater than 1, it is convenient to define the *Reciprocal Spanning-Tree Density of G*, RSTD($G$), as the ratio

$$({}^eC_{(v-1)}) / (t(G)).$$

In general, it is self-evident that

$$STD(G) \leq 1,$$

and

$$RSTD(G) \geq 1.$$

(It is also clear that the only graphs that are not trees for which STD($G$) = RSTD($G$) [= 1] are the circuit-graphs, $C_n$ — see, for example, ref. 29).

We propose that the *Reciprocal Spanning-Tree Density* of a graph $G$  (RSTD($G$)) be defined as a quantitative measure of the *Intricacy* of $G$  — the bigger RSTD($G$) is, the more *intricate* $G$ is. We now investigate this claim by applying these ideas to some well-known and important chemical-graphs. For all the graphs considered we use graph-theoretical notation [30], even though many of these graphs can be used — and, indeed, *are* used — to model chemical structures [28, 31, 32].

## NUMERICAL CALCULATION OF RECIPROCAL SPANNING-TREE DENSITY FOR SEVERAL CLASSES OF GRAPHS

### The Complete Graphs $K_n$

The Complete Graph $K_n$ has every pair of its $n$ vertices joined by a single edge. $K_n$ thus has $(1/2)n(n-1)$ edges in total, and each individual vertex has precisely $(n-1)$ edges incident upon it. $K_n$ is thus a *regular* graph (because every vertex has the same number of edges incident upon it) of *degree* $(n-1)$ (because that is the common number of edges incident upon each vertex). The number of spanning trees, $t(K_n)$, in $K_n$, is given by the Sylvester-Borchardt-Cayley formula [33–35]:

$$t(K_n) = n^{n-2}$$

Thus:

$$\text{RSTD}(K_n) = {}^{(1/2)n(n-1)}C_{(n-1)} / n^{n-2}$$

Application of this formula to $K_5$ is shown in Figure 1. $K_5$ is a complete, non-planar graph of *genus* [36,37] 1 and degree 4. The generalised Euler Theorem for a connected graph is: $v - e + f = 2 - 2g$, where $g$ stands for the genus [36,37] of $G$ and $f$ is the number of *faces* [38] of $G$. With $g=1$, this leads to $v - e + f = 0$.

Because the singular relevance of $K_5$ was first emphasised by Kuratowski in the course of his classic work [39] on characterising non-planar graphs, it is often known as the Kuratowski Graph.
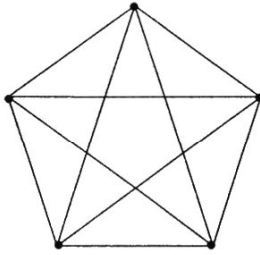


$$t(K_5) = 5^{5-2} = 125$$

$${}^{10}C_4 = 210$$

$$\text{RSTD}(K_5) = 1.68$$

$K_5$

FIGURE 1. Calculation of RSTD($K_5$).

It should be noted that RSTD($K_n$) increases with $n$; for example, RSTD($K_4$) = 1.25 (to three significant figures) whilst RSTD($K_8$) — $K_8$ being [36] of genus 2 — is, to the same accuracy, 4.52. Thus, the *intricacy* of the complete graphs, $K_n$ — at least, as measured by the new index RSTD($K_n$) — does appear to increase with size.

**The Complete Bipartite Graphs $K_{m,n}$**

The Complete Bipartite Graph $K_{m,n}$ is a graph with ($m+n$) vertices that are partitioned into two sets in the following way: none of the $m$ vertices in one set is joined

by an edge to another in the same set, and none of the $n$ vertices in the other set is joined by an edge to a vertex in its own set; however, each of the $m$ vertices in the one set *is* joined by a single edge to every one of the $n$ vertices in the other set. Sometimes, these two vertex sets are thought of as being *coloured*; thus, if the first set of $m$ vertices were coloured red, and the $n$ vertices in the other set were coloured blue, no red vertex would be joined to another red vertex, and no two blue vertices would be connected by an edge; however, each and every pair of red and blue vertices *would* be joined by exactly one edge. $K_{m,n}$ thus has $(m+n)$ vertices and $mn$ edges. The number of spanning trees in $K_{m,n}$ is given by the formula [40,41]:

$$t(K_{m,n}) = m^{n-1} \times n^{m-1}$$

Thus:

$$\text{RSTD}(K_{m,n}) = {}^{mn}C_{m+n-1} / (m^{n-1} \times n^{m-1})$$

This formula is applied to $K_{3,3}$, (the 'Utilities Graph' — see, for example, ref. 42 and p. 142 of ref. 43), in Figure 2. $K_{3,3}$ is a non-planar graph of genus 1 [44,45] and degree 3 for which (as with $K_5$, above) Euler's Theorem requires that $v - e + f = 0$. Kuratowski [39] likewise drew attention to the central importance of $K_{3,3}$ in the context of his pioneering algorithmic approaches to the question of distinguishing between planar and non-planar graphs.
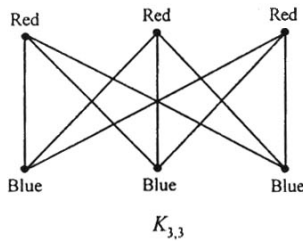


$t(K_{3,3}) = 3^{3-1} \times 3^{3-1} = 81$

$^9C_5 = 126$

$\text{RSTD}(K_{3,3}) = 1.56$

FIGURE 2. Calculation of RSTD($K_{3,3}$).

## The Petersen Graph

The Petersen Graph (Figure 3) is a regular graph of degree 3 that was introduced [46] into Mathematics as a counter-example to a conjecture that Tait made [47] in connection with the Four-Colour Problem [48]. It has had a relevance elsewhere in Mathematics [49] and it also appears to be one of the more important graphs in Chemistry, in which context it depicts possible routes for the isomerisation of trigonal-bipyramidal complexes [50,51].
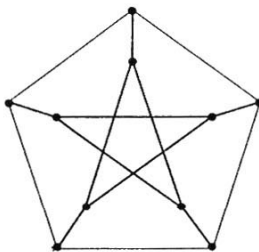


FIGURE 3. The Petersen Graph.

The number of spanning trees in the Petersen Graph is precisely [52,53,40] 2000. (This has been independently verified by at least three unconnected calculations [52,53,40]; the value given on p. 892 of ref. 22 is thus conceded to be in error; all other numerical data from this source that are needed for the present work have been independently checked by us). Also, for the Petersen Graph, $v=10$, $e=15$. Thus: RSTD(Petersen Graph) = $^{15}C_9$ / 2000 = 2.50 (to three significant figures).

## The Blanuša Graph

The Blanuša Graph (see Figure 4) was also introduced in the context of the Four-Colour Problem [54]. Like the Petersen Graph, it is regular of degree 3 and it can in fact be obtained by suitably combining two copies of the Petersen Graph [22].
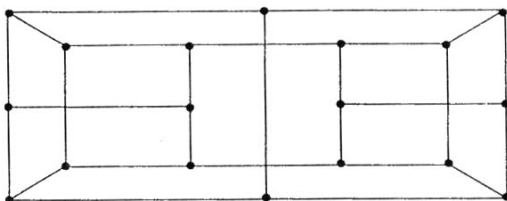
FIGURE 4. The Blanuša Graph.

It is known [22,55] that $t$(Blanuša Graph) = 1037136; also, for this graph, $e$=26 and $v$=18, and so RSTD(Blanuša Graph) = $^{26}C_{17}$ / 1037136 = 3.01 (to three significant figures). It can be seen merely by inspection that the Blanuša Graph is intuitively a more 'complicated' structure than the Petersen Graph, and this impression is confirmed both by the respective number of spanning trees and the reciprocal spanning-tree densities of these two graphs.

### The Desargues-Levy Graph

Like the Petersen and Blanuša Graphs, the Desargues-Levy Graph (Figure 5) is a three-connected, regular graph that has also found chemical application, this time describing isomerisations and rearrangements [51,56–59].
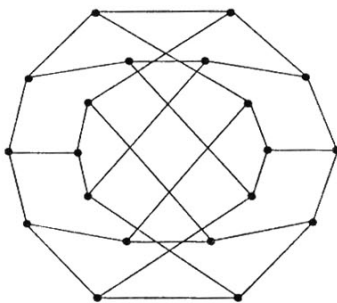


FIGURE 5. The Desargues-Levy Graph.

From the previous work of one of us [22], $t$(Desargues-Levy Graph) = 6144000 and, for this graph, $e$=30 and $v$=20. Thus: RSTD(Desargues-Levy Graph) = $^{30}C_{19}$ / 6144000 = 8.89 (to three significant figures). By this criterion, it thus appears that the Desargues-Levy Graph is more 'complicated' than the Blanuša Graph. This deduction is qualitatively consistent with the respective spanning-tree counts for the two graphs and the impression intuitively gleaned by a visual inspection of their structures.

**Platonic Solids**

The Platonic solids (tetrahedron (**T**), cube (**C**), octahedron (**O**), icosahedron (**I**), and dodecahedron (**D**)) are depicted, in 'three-dimensional' form, in Figure 6, and their corresponding Schlegel diagrams are shown in Figure 7. We include the Platonic solids in this paper because they are continuously attracting the attention of chemists [60-67], with cubane and dodecahedrane providing experimental realisations, while tetrahedrane remains an interesting possibility ,— the $C_{20}$ fullerene would be dodecahedral, and the icosahedron is realised by $B_{12}H_{12}^{2-}$.
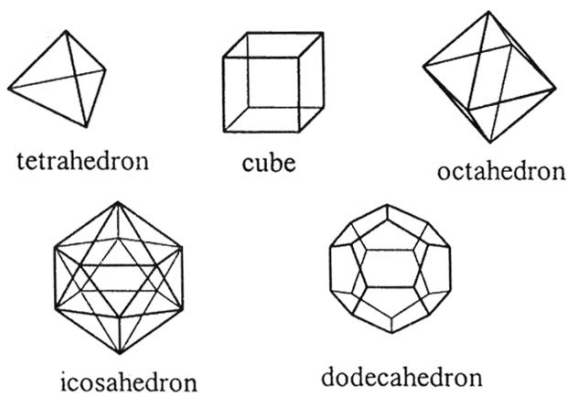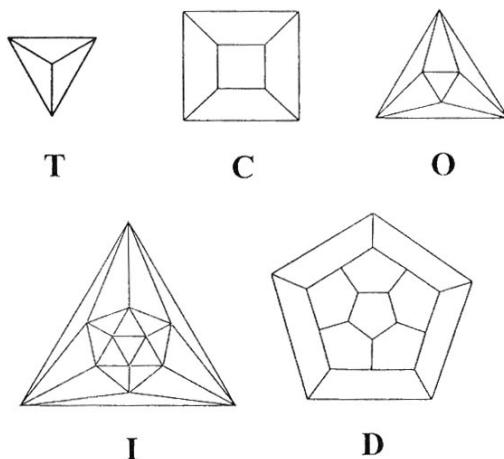


FIGURE 6. The Platonic solids.

FIGURE 7. Schlegel Graphs for the Platonic solids.

The numbers of spanning trees of the Platonic solids are [12,19]: $t(\mathbf{T}) = t(K_4) = 16$; $t(\mathbf{C}) = 384$; $t(\mathbf{O}) = 384$; $t(\mathbf{I}) = 5184000$ and $t(\mathbf{D}) = 5184000$. Furthermore, $^6C_3 = 20$ (for $\mathbf{T}$); $^{12}C_7 = 792$ (for $\mathbf{C}$); $^{12}C_5 = 792$ (for $\mathbf{O}$); $^{30}C_{11} = 54627300$ (for $\mathbf{I}$); and $^{30}C_{19} = 54627300$ (for $\mathbf{D}$). The RSTD-values (to three significant figures) for the Platonic solids are thus: RSTD($\mathbf{T}$) = 1.25; RSTD($\mathbf{C}$) = RSTD($\mathbf{O}$) = 2.06; RSTD($\mathbf{I}$) = RSTD($\mathbf{D}$) = 10.54. It is not surprising that $t(G)$, $^eC_{v-1}$ and the RSTD-values in the cube and the octahedron on the one hand, and in the icosahedron and dodecahedron on the other, are identical, within each pair. The graphs that comprise each of these two pairs are duals of each other. The RSTD-index thus orders the Platonic solids in the following way: $\mathbf{T} < \mathbf{C} = \mathbf{O} < \mathbf{I} = \mathbf{D}$.

The same order is obtained, for example, by the sum of vertex-degrees (or, equivalently, twice the number, $e$, of edges); the sums of the vertex-degrees are given in brackets: $\mathbf{T}(12) < \mathbf{C}(24) = \mathbf{O}(24) < \mathbf{I}(60) = \mathbf{D}(60)$. Certain other quantities, such as, for example, the cyclomatic number [68] and the Bertz complexity-index [2], order the Platonic solids differently: $\mathbf{T} < \mathbf{C} < \mathbf{O} < \mathbf{D} < \mathbf{I}$.

## $C_{60}$ and $C_{70}$ Fullerenes

Buckminsterfullerene, $C_{60}$, (see Figure 8) is selected because of the current interest in the properties of fullerenes and other nano-materials made of carbon atoms [69].
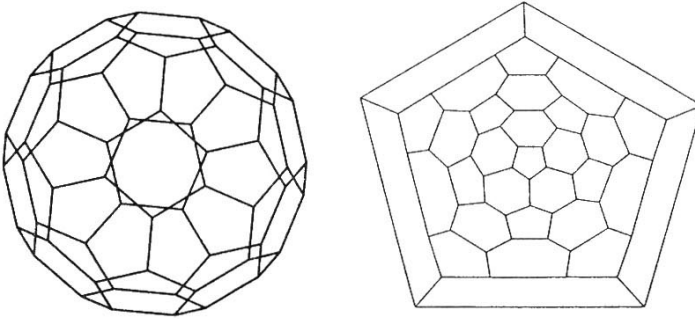


FIGURE 8. Buckminsterfullerene and its Schlegel graph.

There are 1812 $C_{60}$ isomers [70–74]; Buckminsterfullerene is predicted to be the most stable isomer [72,73] and, furthermore, of all these isomers, Buckminsterfullerene is the most nearly spherical. That is to say, the truncated-icosahedral structure is the most uniformly 'curved' of all the $C_{60}$ fullerenes, and, indeed, of all the fullerenes, $C_n$, for a suitable range of $n$ near 60 [75]. There are 8149 $C_{70}$ isomers [70–74]. The stable $C_{70}$ isomer and its Schlegel graph are depicted in Figure 9, and the results for both $C_{60}$ and $C_{70}$ are presented in Table 1; (all numbers quoted are corrected to three significant figures; the sources of the spanning-tree data are refs. 15, 18 and 20).

TABLE 1. Numbers of spanning trees ($t(G)$), values of $^eC_{\nu-1}$, and reciprocal spanning-tree densities (RSTD($G$)) of the $C_{60}$ and $C_{70}$ fullerenes shown in Figures 8 and 9.

| Fullerene | $t$(Fullerene) | $^eC_{\nu-1}$ | RSTD(Fullerene) |
|---|---|---|---|
| $C_{60}$ | $3.75 \times 10^{20}$ | $^{90}C_{59} \approx 1.30 \times 10^{24}$ | 3500 |
| $C_{70}$ | $1.14 \times 10^{24}$ | $^{105}C_{69} \approx 1.70 \times 10^{28}$ | 15000 |

The RSTD-values indicate that $C_{70}$ is a more complicated structure than $C_{60}$. This is also supported, for example, by the fact that the cyclomatic number [68] of $C_{70}$ ($\mu=36$) is bigger than that for $C_{60}$ ($\mu=31$).
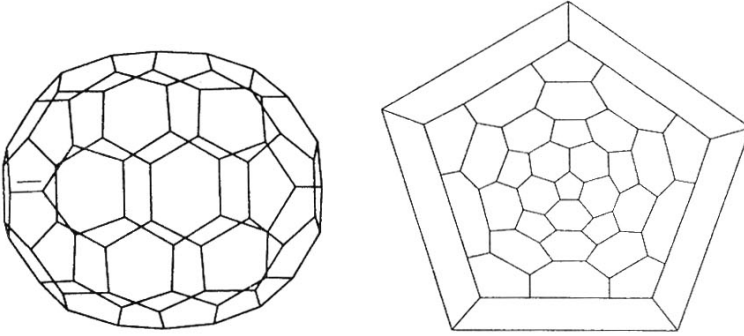
FIGURE 9.  $C_{70}$ and its Schlegel graph.

## All Connected Cyclic Graphs with Five Vertices

We include this set of cyclic graphs because they have already been studied, by Randić [76] and others [77]; all connected cyclic-graphs with five vertices are illustrated in Figure 10.
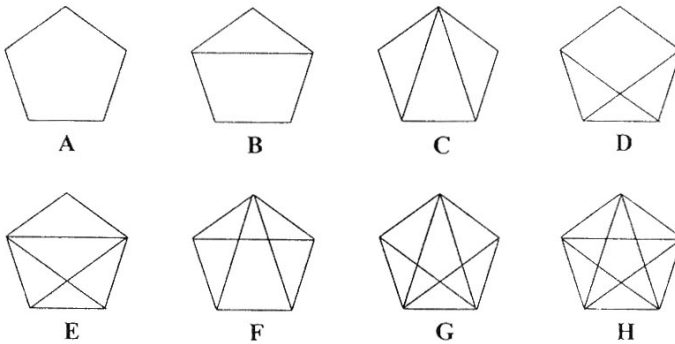
FIGURE 10.  All connected cyclic-graphs with five vertices.

In Table 2 we give the numbers of spanning trees, $t(G)$, the values of $^eC_{\nu-1}$, and the reciprocal spanning-tree densities, RSTD$(G)$, of the cyclic graphs with five vertices, shown in Figure 10 and labelled there as **A** to **H**.

TABLE 2. Numbers of spanning trees ($t(G)$), values of $^eC_{\nu-1}$, and reciprocal spanning-tree densities (RSTD$(G)$; to 3 significant figures) of all connected cyclic-graphs with five vertices; the graphs in question are labelled **A** to **H** and are depicted in Figure 10

| Graph, $G$ | $t(G)$ | $^eC_{\nu-1}$ | RSTD$(G)$ |
|------------|--------|---------------|-----------|
| **A** | 5 | 5 | 1 |
| **B** | 11 | 15 | 1.36 |
| **C** | 21 | 35 | 1.67 |
| **D** | 24 | 35 | 1.46 |
| **E** | 40 | 70 | 1.75 |
| **F** | 45 | 70 | 1.56 |
| **G** | 75 | 126 | 1.68 |
| **H** | 125 | 210 | 1.68 · |

The $t(G)$, $^eC_{\nu-1}$, and RSTD$(G)$ indices ordered the five-vertex cyclic-graphs as follows:

$t(G)$:  **A < B < C < D < E < F < G < H**

$^eC_{\nu-1}$:  **A < B < C = D < E = F < G < H**

RSTD$(G)$:  **A < B < D < F < C < G = H < E**

It will be observed that each of these quantities has produced a different order. That given by RSTD$(G)$ is somewhat implausible; the order obtained *via* $t(G)$ is intuitively acceptable, as is that given by $^eC_{\nu-1}$.

In Table 3 we offer a number of other indices, taken from ref. 77, for the graphs of Figure 10. The indices considered are the Wiener index (W) [78], the Balaban indices (J, $J_\Omega$) [77,79], the Wiener-sum index (WS) [76,77,80] and the two Kirchhoff indices (Kf, KfS) [77,81].

TABLE 3. The Wiener indices (W), Balaban indices (J, $J_\Omega$), Kirchhoff indices (Kf), Wiener-sums (WS) and Kirchhoff-sums (KfS) for the eight five-vertex cyclic-graphs of Figure 10. (All non-integral data are presented corrected to three places of decimals.)

| Graph, $G$ | $-W$ | J | $J_\Omega$ | $-Kf$ | WS | $-KfS$ |
|---|---|---|---|---|---|---|
| **A** | $-15$ | 2.083 | 3.125 | $-10.000$ | 14.583 | $-7.000$ |
| **B** | $-14$ | 2.194 | 3.789 | $-8.812$ | 16.886 | $-6.091$ |
| **C** | $-13$ | 2.486 | 4.664 | $-6.952$ | 18.583 | $-5.476$ |
| **D** | $-13$ | 2.389 | 4.866 | $-6.417$ | 19.956 | $-5.208$ |
| **E** | $-12$ | 2.804 | 5.849 | $-5.750$ | 20.826 | $-4.875$ |
| **F** | $-12$ | 2.711 | 6.067 | $-5.333$ | 22.071 | $-4.667$ |
| **G** | $-11$ | 3.138 | 7.351 | $-4.667$ | 23.357 | $-4.333$ |
| **H** | $-10$ | 3.571 | 8.929 | $-4.000$ | 25.000 | $-4.000$ |

The above Table gives rise to the following orderings for the intricacies of the eight five-vertex cyclic-graphs, **A** to **H**, shown in Figure 10:

$-W$           : **A** < **B** < **C** = **D** < **E** = **F** < **G** < **H**

J              : **A** < **B** < **D** < **C** < **F** < **E** < **G** < **H**

$J_\Omega$ & WS  : **A** < **B** < **C** < **D** < **E** < **F** < **G** < **H**

$-Kf$ & $-KfS$ :  **A** < **B** < **C** < **D** < **E** < **F** < **G** < **H**

Amongst these indices, $J_\Omega$, WS, $-Kf$ and $-KfS$ gave rise to the same ordering of these eight five-vertex cyclic-graphs, as did $t(G)$. This result also agrees with Randić's ordering for the same octet of five-vertex cyclic-graphs [76]. His order was based on the Wiener-sum indices derived from the quotient matrix, denoted "$D/\Delta$", in which the elements of **D**, the distance matrix, are divided by the corresponding off-diagonal elements of $\Delta$, the detour matrix [82,83]. The negative of the Wiener index supports the order given by $^eC_{\nu-1}$. The same ordering is also obtained by the vertex-degree sums (or, equivalently, as has already been observed, twice the number of

edges, $e$ (given in brackets)): $A(10) < B(12) < C(14) = D(14) < E(16) = F(16) <$ $G(18) < H(20)$. If, however, we consider only the sums of the vertex-degrees higher than 2, the following order emerges: $A(0) < B(6) < C(10) < D(12) < E(14) < F(16) <$ $G(18) < H(20)$, which fully agrees with the orderings obtained by means of $t(G)$, $J_\Omega$, WS, $-$Kf, and $-$KfS.

## CONCLUDING REMARKS

As is illustrated in the above applications of several 'intricacy indices' to the five-vertex cyclic-graphs **A** to **H** of Figure 10, by no means all of the indices proposed for assessing the intricacy of a graph necessarily agree among themselves when they are applied to a specific collection of graphs whose 'intricacy' it is desired to quantify — or, at the very least, to order. This, though, need not, we feel, give cause for undue concern; the intricacy of a graph is, after all, a somewhat *fuzzy* concept [84–87] and how it is defined will naturally determine the *order* of such intricacy decided upon within any given set of (molecular) graphs. Bonchev and Seitz, on p. 354 of ref. 87, stated the opinion that "...there are different kinds of complexity and no single concept could embrace all the aspects..." of it. Nevertheless, the reciprocal spanning-tree density is, we submit, *a physically and intuitively sensible approach to this problem*, representing, as it does, the *reciprocal* of the *probability* that if *any* set of $(v-1)$ edges is selected in a graph that comprises $v$ vertices, and the other $(e-v+1)$ edges are deleted, the resulting entity is a spanning tree.

In our initial evaluation of this newly proposed 'reciprocal spanning-tree density', $RSTD(G)$, as an index for quantifying the intricacy of a cyclic graph $G$, our emphasis after introducing it has been almost entirely on numerical computations and applications of it. In conclusion, though, we just mention in passing that, for certain categories of graphs (such as, for example, the Complete Graphs $K_n$ and the Complete Bipartite Graphs $K_{m,n}$, encountered above), it is possible to derive general formulae for $RSTD(G)$. Thus — as already pointed out — it is, for instance, easy to show that

$$RSTD(K_n) = \{^{(1/2)n(n-1)}C_{n-1}\} \,/\, \{n^{n-2}\}$$

and that

$$RSTD(K_{m,n}) = \{^{mn}C_{m+n-1}\} \,/\, \{m^{n-1} \times n^{m-1}\}.$$

It is clear that analogous formulae could always be derived for any class of graphs whose spanning-tree counts can be obtained in closed form. One advantage of casting the results like this would be that there is then the possibility of seeing how the RSTD($G$) index within a given class of graphs behaves as the graphs get bigger — and, in the limit, when $n$, $m$,...etc. $\to \infty$. The index RSTD($G$) is thus here offered for possible further evaluation, investigation and assessment — both numerical and algebraical.

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where the curly-bracket notation, $\{x\}$, denotes 'the smallest integer not less than $x$'. For example, $g(K_5)=\{(1/12)\ (5-3)\ (5-4)\}= \{(1/6)\} = 1$. The above formula is discussed, for instance, in ref. 30 (p. 118) and in ref. 27 (p. 71), and is proved in ref. 37.

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where, as in ref. 36, the curly-bracket notation, $\{x\}$, denotes 'the smallest integer not less than $x$'. For example, $g(K_{3,3}) = \{(1/4) \ (3-2) \ (3-2)\} = \{(1/4)\} = 1$.

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