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On topological form in structures

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This paper begins with a review of the Euler relation for the polyhedra and presents the corresponding Schläfli relation in n, the polygonality, and p, the connectivity of the polyhedra. The use of ordered pairs as given by (n, p), the Schläfli symbols, to organize the mapping of the polyhedra and its extension into the two-dimensional (2D) and three-dimensional (3D) networks is described. The topological form index, represented by l, is introduced and is defined as the ratio of the polygonality, n, to the connectivity, p, in a structure, it is given by $l = n/p$. Next a discussion is given of establishing a conventional metric of length in order to compare topological properties of the polyhedra and networks in 2D and 3D. A fundamental structural metric is assumed for the polyhedra. The metric for the polyhedra is, in turn, used to establish a metric for tilings in the Euclidean plane. The metrics for the polyhedra and 2D plane are used to establish a metric for networks in 3D. Once the metrics have been established, a conjecture is introduced, based upon the metrics assumed, that the area of the elementary polygonal circuit in the polyhedra and 2D and 3D networks is proportional to a function of the topological form index, l, for these structures. Data of the form indexes and the corresponding elementary polygonal circuit areas, for a selection of polyhedra and 2D and 3D networks is tabulated, and the results of a least squares regression analysis of the data plotted in a Cartesian space are reported. From the regression analysis it is seen that a quadratic in l, the form index, successfully correlates with the corresponding elementary polygonal circuit area data of the polyhedra and 2D and 3D networks. A brief discussion of the evident rigorousness of the Schläfli indexes (n, p) over all the polyhedra and 2D and 3D networks, based upon the correlation of the topological form index with elementary polygonal circuit area in these structures, and the suggestion that an Euler–Schläfli relation for the 2D and 3D networks, is possible, in terms of the Schläfli indexes, concludes the paper.

KEY WORDS: chemical topology, polyhedra, Euler relation, Schläfi symbol

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1. Introduction

Euler's relation between the number of vertices, V, edges, E, and faces, F, of convex polyhedra was developed in the middle of the 18th century and its discovery marks the origin of the discipline of topology [1]. This relation is shown in equation (1) below:

$$V - E + F = 2. \tag{1}$$

From this equation it is said that the Euler characteristic for the sphere is 2. This simply, and elegantly, means that any division of a sphere into vertices, edges and faces will have that combination so specified in equation (1). It happens that the convex polyhedra, with all their inherent symmetry and external beauty, are the idealized divisions of the sphere into the topology suggested first by Euler in his 1758 paper [1].

During the 19th century, a paper due to Schläfli was published [2] in which the identities shown in equations (2) and (3) were discovered:

$$\mathrm{n}F = 2E. \tag{2}$$

$$\mathrm{p}V = 2E. \tag{3}$$

Schläfli identified the polygonality, n, of convex polyhedra as the averaged number of sides of the polygonal faces in an object derived from truncation of the sphere. He determined the relation shown in 2 which states that the averaged polygonality in such an object, n, multiplied by its number of faces, F, is equal to twice its number of edges, E. Because each edge, E, is shared by two faces (i.e. adjacent faces share a common edge) this relationship is rigorous.

Similarly in 3 we see that Schläfli identified a relationship between the connectivity, p, of convex polyhedra and the number of vertices, V, and edges, E. The connectivity, p, is identified as the averaged number of edges meeting at each vertex of a polyhedron. Because each edge terminates at two vertices, one can see that this Schläfli relation is rigorous. One speaks of averaged numbers for n and p, because unless the polyhedron is regular (meaning all faces are identical polygons, as given by the five Platonic solids) there can be differing numbers of edges, E, to each polygonal face, and/or differing numbers of edges, E, that meet at each polygonal vertex in the given polyhedron. One can therefore identify the semi-regular polyhedra, these are the Archimedean polyhedra (with more than one type of polygonal face) and Catalan polyhedra (with more than one type of polygonal vertex) [3,4]. There are, in addition, innumerable irregular polyhedra, these are polyhedra in which there is more than one type of polygonal face *and* more than one type of polygonal vertex. The irregular polyhedra have been reported as recently the beginning of the 21st century.

Schläfli substituted equations (2) and (3) into the Euler relation, as is shown in equation (4), to obtain a relation between V, E and F, known as the primary topological indexes, and n and p, known as the secondary topological indexes.

$$\frac{1}{\mathrm{n}} - \frac{1}{2} + \frac{1}{\mathrm{p}} = \frac{1}{E}. \tag{4}$$

Among other reasons, this latter Schläfli relation is important from the perspective of the Schläfli symbols (n, p) that can be identified for any structure. All of the convex polyhedra have rigorously determined values of n and p, just as in the case of the primary topological indexes identified for them and given by V, E and F. The ordered pair thus formed, (n, p), the Schläfli symbol, represents a location in a Cartesian-like space, called a Schläfli space, in which the polyhedral object can be mapped.

The beginnings of this topological mapping for the regular polyhedra have been shown elsewhere [3]. As a Cartesian-like space, the map is outlined by increasing connectivity, p, running as an axis from left to right in the map, and by increasing polygonality, n, running as an axis from top to bottom in the map. The five regular polyhedra are called the Platonic solids for their role as Elements in Plato's philosophical treatise known as the Timeas [4]. The Platonic solid with the highest topology (as defined here by its position in the topology map) is the tetrahedron (meaning it has four equivalent faces) with the Schläfli symbol (3, 3). It marks the origin of this map. Similarly, lining the column underneath the tetrahedron, there is the cube (4, 3) and the pentagonal dodecahedron (5, 3). And to the right of (3, 3), are the octahedron (3, 4) and the icosahedron (3, 5).

One can immediately see the power of the Schläfli relation as an organizing principle in its usefulness as a mapping tool for determining the identity and relative location of all of the various polyhedra. One could extend this mapping to include the semi-regular and irregular polyhedra as well. The Archimedean polyhedra have fractional polygonality n, while the Catalan polyhedra have fractional connectivity p, and the irregular polyhedra have both fractional polygonality and fractional connectivity in their Schläfli symbol (n, p).

During the 1950s A.F. Wells began his enumerative work on two-dimensional (2D) and three-dimensional (3D) networks and novel crystal structures [3]. He labeled these novel networks with their corresponding Schläfli symbols (n, p) to map and identify them. For while Wells did not determine a Schläfli-like relation for 2D and 3D structural patterns (that is collections of vertices, edges and faces filling 2D and 3D space, and not constrained to the surface of a sphere) he nonetheless discovered that both the polygonality, n, and the connectivity, p, could be rigorously calculated within the corresponding units of pattern of extended structures in both 2- and 3-dimensions [3]. He properly concluded that the topology map for the polyhedra could be extended in the space of n and p, the Schläfli space, by a simple augmentation of the ordered pairs of numbers (n, p), to the right and downwards from the Schläfli symbols for the polyhedra. From the original polyhedral topology map of Wells [3], an augmentation of this map involved moving into frontier that included the various 2D tessellations, like the regular 2D extended structures of the honeycomb net (6, 3), the square net (4, 4) and also the closest packed net (3, 6), and on to include the semi-regular and irregular tessellations of the Euclidean plane. Beyond the 2D nets, the map extended further to the right and downward into the territory of the regular, semi-regular and irregular 3D networks. The extension of the topology map, due to A.F. Wells, has been shown elsewhere [5]. Note that to the right of the 2D networks, the frontier of the 3D nets, a given Schläfli symbol (n, p) may represent more than one way of filling space with a network of the specified topology, so that one may have the potential for topological isomerism in 3D.

Early on in the 1950s, work by Wells involved the enumeration of regular 2D and 3D networks, that is networks in which the polygonality of circuits in the net is a uniform number, and the connectivity of the vertices in the networks is a uniform number. These networks represent structures with some of the highest topologies possible, and the work included such topologies as that represented by the Schläfli symbol (7, 3). Particularly in this instance, according to Wells, he was attempting to extend the topology map from the index (5, 3), the Platonic solid called the pentagonal dodecahedron, to (6, 3), the 2D tessellation which is known as the honeycomb net, onto (7, 3) which represents a continuation of this sequence into 3D space. He eventually determined four distinct structures that possessed the Schläfli symbol (7, 3) [3]. These four structures with the same the Schläfli symbol (7, 3), thus constituted one of the first examples of topological isomerism ever reported. He did other similar elegant work on 3D networks of topology (8, 3), (9, 3), (10, 3) and (12, 3) [3]. Later on, as well as continuing his study of regular networks, in addition Wells turned to networks whose topology was lowered, these were the semi-regular and irregular 3D networks [6].

The theme for the purpose of the present discussion, is to establish a relation between these topological Schläfli indexes, introduced and described above, and the elementary polygonal circuit area in a structure, labeled as area(n, p). The structures considered in this analysis include polyhedra, the 2D tessellations and the 3D networks. The reasons for choosing elementary polygonal circuit area in order to establish a geometrical–topological correlation in structures will be discussed more fully below in connection with the concept of a structural metric. It has been discovered, in the present work, that one can formulate a topological index derived from n and p that correlates with the elementary polygonal circuit area of structures, to include the polyhedra and the 2D and 3D patterns. This new index, first described in 1997 [5], is defined as the ratio of the polygonality to the connectivity in a given structure, l. This is shown in equation (5):

$$\mathrm{l} = \frac{\mathrm{n}}{\mathrm{p}} \tag{5}$$

Such a topological index of structures is a measure of what is termed the compactness of a structure, as described below, it is hereafter called the Schläfli topological form index.

2. Identification of a geometrical standard

In order to establish a correlation between a geometrical structural parameter and a topological structural parameter, in patterns, it is necessary to define a standard of length, called a metric, amongst which all structures in the same class, i.e. in the class of the polyhedra or in the class of the 2D tessellations or in the class of the 3D networks, possess the metric commonly. Establishing these metrics of length is essential to identify property correlations across structures in all classes and, of the utmost importance, it provides an internal consistency in the correlation analysis. In this section, we will postulate a metric for the polyhedra, called the Wells polyhedra metric [7], and from which the metric for the 2D structures and the metric for the 3D structures are derived. Purposely, the derivation of the metrics in 2D and 3D will be posited with the concomitant inference that they will so support the geometrical–topological correlation established at the end of the paper.

Before moving on to the discussion of metrics, it is important to clarify why the geometrical–topological structural correlation being described in this paper involves the geometrical structural parameter of elementary polygonal circuit area. In the course of this investigation, the problem arose as to how one could establish the applicability of the Schläfli symbols to the 2D and 3D networks. As has been discussed in the previous Section, A.F. Wells found that he could calculate the Schläfli indexes (n, p) for any 2D or 3D pattern, but the Schläfli relation given in equation (4) in this paper was not rigorous for these ordered pairs (n, p) associated with patterns in higher dimension than the polyhedra.

It is the purpose of the present communication to establish a different relation involving the Schläfli indexes and another property of structures, this being the geometrical structural property of elementary polygonal circuit area, in order to demonstrate that these topological indexes have applicability to the rigorous analysis of mathematical properties of the 2D and 3D networks. This may have importance with respect to the eventual formulation of an Euler–Schläfli relation for the 2D and 3D structures. Beyond this, such a study as the present one has as its goal to show the reader that topological indexes of structures have a bearing on, and are related to, geometrical properties of structures.

In a separate sense, the choice of elementary polygonal circuit area as a geometrical structural property used to establish a geometrical–topological correlation, was made on the basis that 2D patterns have polygonal circuit area but, technically, no volume, and further that this structural property of polygonal circuit area is shared with the polyhedra and the 3D structures. Also, there are additional reasons, connected with the problem of establishing a suitable metric, for not employing geometrical structural volume in a correlation with topological structural parameters. These will not be discussed here. At any event, in the polyhedra and 2D and 3D patterns one can determine (even if this involves an averaging process, as in the case of the semi-regular and irregular structures) the elementary polygonal circuit area, labeled as area(n, p), of a structure.

Turning to the identification of a fundamental geometrical structural parameter, a metric of length, in order to provide a basis for a geometrical–topological correlation, the original work of Euler is considered [1]. Euler envisioned the inscription of the polyhedra inside the sphere, in order to establish the relation shown in equation (1) in the previous section. In the interest of establishing suitable metrics for the 2D and 3D patterns, we begin with the assumption that the polyhedra are inscribed in the unit sphere. Therefore, from the center of the sphere, and the corresponding polyhedra inscribed therein, there exist radii of length unity, that point in all directions about the sphere (polyhedra), including into the vertices of the various polyhedra. This particular assumption is the basis for the calculation of the edge lengths and face areas of the polyhedra, and the results of this analysis are later used to establish metrics for the 2D and 3D patterns. The assumption that the polyhedra are inscribed in the unit sphere, is therefore called the Wells fundamental polyhedra metric [7].

The analysis of edge lengths and face areas, to eventually be used in the geometrical–topological correlation, begins with the inscription of the regular tetrahedron (3, 3) in the unit sphere. It is an easy matter to calculate the corresponding edge of this polyhedron, one uses plane geometry and the fact that the unit radii pointing into a pair of tetrahedral vertices form an obtuse isosceles triangle in which the obtuse angle is ideal at 109.47°. From this one gets an edge of $2\sqrt{2}/\sqrt{3}$ and a corresponding face area given as $2/\sqrt{3}$. Turning next to the cube (4, 3), unit radii pointing into adjacent vertices form a right triangle possessing a hypotenuse of length 2, comprised of the corresponding face diagonal, leading to an edge length of $2/\sqrt{3}$ and a face area of 4/3. Turning to the octahedron (3, 4), unit radii pointing to an axial and an equatorial pair of vertices define an isosceles right triangle that leads to an octahedral edge of $\sqrt{2}$ and an octahedral face area of $\sqrt{3}/2$.

The two other regular (Platonic) polyhedra, the pentagonal dodecahedron (5, 3) and the triangular icosahedron (3, 5) present esoteric geometrical problems, and they are not essential to further establish the 2D and 3D metrics, so their analysis will be left to a separate paper. From the preceding paragraph, all the information required in order to establish the 2D and 3D metrics, and the corresponding conjecture that forms the basis of the geometrical–topological correlation proposed later in this paper, is available, upon positing a couple further assumptions. One should bear in mind that the metric for the polyhedra is provided through the assumption that they are inscribed in the unit sphere. This leads to different edge lengths and different face areas in each of the polyhedra, however they share their inscription on the unit sphere, which is the metric of length for them. From this analysis, it is clear that they must, in fact, have different face areas, and the following relations hold: area(5, 3) > area(4, 3) > area(3, 3) > area(3, 4) > area(3, 5). These latter relations are a consequence of the equation between the form index, l, and the elementary polygonal circuit area, symbolized by area(n, p), which will be proposed and developed later in the paper.

To identify the metric for the 2D tessellations, one looks to the Schläfli indexes in 2D and in the polyhedra to see if any structures between the 2 classes possess identical form indexes, l. For if corresponding structures between the polyhedral class and the class of 2D tessellations possess the same topological form index, l, they must possess the same elementary polygonal circuit area, area(n, p). That this must be so, is based upon the requirement of providing internal consistency with the geometrical–topological relation assumed to hold for structures in the development of this paper. Such an assumption as this one supports the latter conjecture and is thereby consistent with it. Such a relationship as this, called the Wells structural correspondence principle [7], upon which the identity of the metric in 2D structures is based, represents a 2nd assumption introduced in this paper. Its converse would be simply inconsistent with the geometrical–topological conjecture introduced later in the paper. The square net (4, 4) has a form index of unity, which is the same as the form index in the tetrahedron (3, 3). The regular square net (4, 4) and the tetrahedron (3, 3) have been illustrated elsewhere [3, 4]. Therefore, the 2D metric is established as the corresponding edge length of the square face of the square net, which has the same face area as the tetrahedron inscribed in the unit sphere. As a consequence the following relation, shown in equation (6), holds:

$$\text{area}(3,3) = \text{area}(4,4) = 2/\sqrt{3}. \tag{6}$$

And the corresponding 2D metric is just the edge of the square in (4, 4), or $\sqrt{2/\sqrt{3}}$.

To get the edge metric in 3D, we turn to the related morphologies of the cube (4, 3), the square net (4, 4) and the primitive cubic net (4, 6), these have been discussed and illustrated elsewhere [3, 4]. It is a 3rd, and final, assumption, introduced in this paper, that structures of related morphologies in different structural classes have face areas that are proportional. This is called the Wells morphological principle [7]. The cube, with the Schläfli symbol (4, 3), the square net (4, 4), and the primitive cubic net (rocksalt structure-type) (4, 6), all share perfectly square faces as a common morphological theme in their structures. Therefore on the basis of the morphological principle, we can write the following proportionality expression down:

$$\frac{\text{area}_{(4,3)}}{\text{area}_{(4,4)}} = \frac{\text{area}_{(4,4)}}{\text{area}_{(4,6)}}. \tag{7}$$

By substitution the unknown in 7, area(4, 6), can be solved for as is shown in 8.

$$\text{area}_{(4,6)} = \text{area}_{(4,4)} \left(\frac{\text{area}_{(4,4)}}{\text{area}_{4,3)}} \right) = \text{unity}. \tag{8}$$

It is therefore established in this scheme, developed out of the fundamental assumptions of inscription of the polyhedra on the unit sphere, known hereafter as the Wells polyhedra metric, and the Wells structural correspondence principle described above, and finally the Wells morphological principle, just introduced here, that the metric for all of the 3D networks is unit edge length. This is derived from the fact that the primitive cubic net (rocksalt structure-type) (4, 6) has unit face area and therefore unity for its edge length. Therefore, all the edges of all of the circuits in the 3D nets share edge length unity for the purposes of providing a geometrical–topological analysis of structures that is internally consistent.

3. Consequences of the metrics

A representative sampling of 12 structures has been analyzed topologically by identifying the ordered pair (n, p), the Schläfli symbol, and in terms of the elementary polygonal face areas of the structures, symbolized as area(n, p), for use in establishing a geometrical–topological correlation. The set of 12 structures includes the 3 regular polyhedra discussed above, the 3 regular 2D tessellations, 3 regular 3D nets, 1 Archimedean 3D net, 1 Catalan 3D net and 1 irregular (Wellsean) [5] 3D net. This sampling provides a broad base of potential topological varieties of structure from which to determine if a correlation exists between the topological form index, l, of equation (5), and the corresponding elementary polygonal circuit area, labeled area(n, p).

Table 1 provides a compilation of the data for these 12 structures, note that the metric for the polyhedra is inscription on the unit sphere, the resulting edge metric for the 2D tessellations is just $\sqrt{2/\sqrt{3}}$, by application of the Wells structural correspondence principle, and the edge metric of the 3D networks is therefore just unity, by application of the Wells morphological principle. In table 1, the $ThSi_2$ structure-type labeled by the Schläfli symbol (10, 3) [8], the diamond structure-type labeled as (6, 4) [9] and the (primitive cubic net) rocksalt structure-type labeled as (4, 6) [3] are the regular structures, and they possess ideal bond angles. The Cooperite structure-type labeled as $(6^{2/5}, 4)$ [10] is Archimedean, and is assumed to have ideal tetrahedral angles and distorted square planar angles in the calculation of its polygonal circuit area. The Waserite structure-type labeled as (8, 3.4285) [11] is Catalan and has ideal bond angles, and the glitter structure-type with the Schläfli index $(7, 3^{1/3})$ [5] is topologically irregular and has ideal tetrahedral angles and distorted trigonal planar angles assumed in the calculation of its polygonal circuit area.

Table 1
Geometrical–topological data for 12 structures.

Name	(n, p)	l = n/p	Area(n, p)
ccp network	(3, 6)	1/2	1/2
Primitive cubic	(4, 6)	2/3	1
octahedron	(3, 4)	3/4	•3/2
tetrahedron	(3, 3)	1	2/ • 3
square net	(4, 4)	1	2/ • 3
cube	(4, 3)	$1^{1/3}$	$1^{1/3}$
diamond	(6, 4)	$1^{1/2}$	$\sqrt{2/3}$ •
Cooperite (PtS)	$(6^{2/5}, 4)$	$1^{3/5}$	$2\sqrt{2}\pi/3$
honeycomb net	(6, 3)	2	3
glitter	$(7, 3^{1/3})$	$2\pi/3$	$\sqrt{2/\sqrt{3}}$ •
Waserite (Pt_3O_4)	(8, (2/5)e •)	$2^{1/3}$	•2e
$ThSi_2$	(10, 3)	$3^{1/3}$	7•3/2

One can see immediately that the form indexes, l, and the polygonal circuit areas, called area(n, p), are all expressible in closed form as factors of whole numbers, fractions, square roots of simple integers and the mathematical constants π and e. The honeycomb network (6, 3), the structure of the graphene sheet, with an edge length of $\sqrt{2/\sqrt{3}}$, has a hexagonal face area of exactly 3. The diamond structure-type given by (6, 4) and illustrated elsewhere [9], with unity edge length and tetrahedral bond angles, has an elementary polygonal face area of exactly $\sqrt{2/3}$ •. The Waserite structure-type given by (8, 3.4285) and illustrated and discussed previously [11], a Catalan network in 3D, has octagonal elementary polygonal circuits in its structure which have exactly the face area of •2e when the network possesses unity edge length. Finally, the glitter structure-type with Schläfli index $(7, 3^{1/3})$, a topologically irregular network illustrated elsewhere [5], has a form index, l, of 2/3, and an elementary polygonal circuit area (weighted average of 6-gon and 8-gon areas which occur in a 1-to-1 ratio in glitter) consisting of a composite factor that is the edge metric determined for the 2D tesselations, and the mathematical constant π, it is given as $\sqrt{2/\sqrt{3}}$ •.

The existence of closed form numbers, and especially the occurrence of the mathematical constants π and e in the computation of some of the polygonal circuit areas in these structures, is mysterious. Such apparent coincidences are herein termed Wells coincidences [7]. The Wells coincidences suggest that the polygonal circuit area of the chair hexagons in the diamond lattice [9], for instance, is just a scaling of π. They suggest that the area of the eight-sided circuitry in the real Waserite phase [11], Pt_3O_4, is just a scaling of e. The Wells coincidences, therefore, suggest that the structure of crystalline matter is an approximation to Platonic archetypes.

Indeed, it would seem that all the polyhedra, 2D tessellations and 3D networks, perhaps numbering in the 1000s in terms of those observed as pure forms in models of various polyhedra and 2D and 3D structural-types [3, 4], have an eternal, separate existence as Platonic archetypes. The diamond structural-type exists in a perfect form as a Platonic archetype, in which its chair substructures possess unity edge length and have a geometrical area exactly given by $\sqrt{2/3}\,\bullet$, for example. It must not be overlooked in this context that with the three assumptions posited here, and subsequent derivation of the metrics for the polyhedra and the 2D and 3D networks, respectively, provided in this paper, together with the standard crystallographic description of structures in terms of the space group symmetry and the Wyckoff positions of the vertices, and through the use of elementary plane geometry, one can provide a geometric construction of the mathematical constants π and e that complement the innumerable series and product representations of these ubiquitous numbers.

4. The Wells conjecture and geometrical–topological correlation

Data from table 1 has been mapped to a graph in which the topological form index, l, is plotted along the horizontal axis, and the elementary polygonal circuit area is plotted along the vertical axis, for the set of 12 representative structures described above. The empirical plot is shown completely below in figure 1. The data, consisting of the geometrical–topological information on the 12 structures given in the previous section, was fit reasonably well to a quadratic function in l. Least squares regression analysis of the data showed a reliability factor of 0.9764 (a perfect correlation has a reliability factor of 1.000).

The geometrical–topological correlation equation for the 12 structures in the analysis is shown below:

$$\text{area(n, p)} = A.\text{l}^2 + B.\text{l} + C. \tag{9}$$

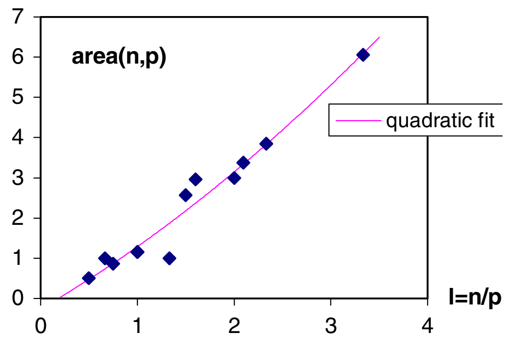

Figure 1. Regression fit of the data in Table 1 representing the elementary polygonal circuit area, area(n, p), versus the topological form, 1, for the 12 structures.

The parameters in equation (9) are given as $A = 0.152$, $B = 1.401$ and $C = -0.265$, these parameters will shift slightly as more geometrical–topological data for the polyhedra, 2D tessellations and 3D networks is obtained and plotted. It is not clear to the authors whether the assumptions introduced earlier in the paper have biased the data towards exhibiting such a strong correlation as is evidenced by the dataset. Also, it is possible, under the assumptions introduced earlier in the paper, to calculate the parameters in equation (9) from corresponding sets of three simultaneous equations, and this direction will be looked into in a separate paper.

The presence of the very strong correlation between the topological form index, l, for structures and their elementary polygonal circuit area, area(n, p), suggests a mathematical conjecture which is called the Wells conjecture [7]. It is stated below:

The elementary polygonal circuit area of a structure, be it a polyhedron, a 2D tessellation or a 3D network, under a suitable metric, is proportional to a function of the topological form index l, which is the ratio of the structure's polygonality, n, to the structure's connectivity, p.

There is no proof of the Wells conjecture presently. It appears that such a proof, if one exists, will be very tenuous and difficult to elucidate, as the correlation described above is only approximate.

The presence of this strong geometrical–topological correlation is quite surprising in that one would not have expected topological parameters, like n and p, which are pure numbers, to be related to a geometrical property of a given structure, like elementary polygonal circuit area. Indeed, the elementary polygonal circuit area of a given structure would seem to have a purely empirical value for a given arbitrary network. This empirical correlation is also fundamental from the point of view of the Schläfli symbols (n, p) as it shows there is a degree of mathematical rigor, evidenced by the strong reliability index of the functional fit of the data, in the Schläfli symbols for the 2D and 3D structures as well as the polyhedra. In this instance we recall that the polyhedra are governed by the Euler–Schläfli relations shown as equations (1) and (4) in this paper. This latter result suggests it may be possible to formulate an Euler–Schläfli relation, using n and p in some functional form, to predict the number of edges occurring in the units of pattern of 2D and 3D structures.

5. Conclusions

In conclusion, we state a note on compactness and the computational scheme for obtaining the topological indexes of arbitrary networks. Earlier it was thought by the authors that the topological form index, l, was a measure of the density of the network. Density is a measure of the number of vertices in a metric of volume of a structure. At this juncture it is not clear that l correlates with density, in fact empirical evidence from hexagonite and the expanded hexagonites [12] suggests strongly that l is not a measure of density. It is suggested here that the term compactness be used with reference to l, compactness is a measure of how tightly connected together (the degree of tautness) the circuitry in a net is held. It is a measure of the compactness of area which is occupied by matter in the structure. Low l correlates with low elementary polygonal circuit area and high compactness, and vice versa.

It is important to point out the significance of equation (9) in terms of the space of all possible networks [3, 4]. Equation (9) represents a set of points through the space of all possible networks (all potential values of the parameter $l = n/p$). It thus identifies those networks with a given set of coordinates in the space (l, area(n, p)) that are potentially realizable in Euclidean space as actual structures. One could propose a network with a given value of (n, p), its associated Schläfli symbol, in which the value of the ordered pair (n, p) for an arbitrary network can be systematically derived from the network's corresponding Wells point symbol (which itself is a straightforward, systematic coding of the topology of a given network from 1st principles of its topology) by a procedure described previously by the authors [13]. From the associated topological symbol (n, p) computed in this way, one can use equations (5) and (9) in this paper, to calculate the corresponding values of such a structure given by the topological form index, l, and the area of the elementary polygonal circuit, area(n, p), respectively.

By plotting the coordinates in this manner as given for example by Figure 1 for the set of 12 structures, one could therefore locate that point in the space represented by the graph of equation (9). If in fact such a point doesn't fall in the proximity of the curve given by equation (9), then the proposed network will probably not be able to be realized in practice in the realm of crystallographic structure-types due to various complicated issues such as residual angle strain or length strain implied in the hypothetical network. Therefore equation (9) represents all potential crystal structures that may be realized in model building (in the spirit of A.F. Wells) or in actual crystallography and is thus a predictive tool for the elucidation of further structures in Euclidean space and their geometrical and topological properties.

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Dedication

This manuscript is dedicated to Joseph Bucknum late of Buckingham, PA. Joseph Bucknum passed away on Christmas Eve, 2001. He was a veteran of World War II and was my Uncle and my Godfather. In my childhood I remember how friendly and full of humor he was as my father Walter Bucknum would take the family from Holland to Yardley to visit with Uncle Joe and Aunt Bette. Aunt Bette is my Godmother. God Bless Joseph Bucknum as he lives out his years in Heaven.

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