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COSMOGONY OF THE MATERIAL WORLD

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Whisper your Faith:

Whisper your faith, in dark, secret fear have me no longer of a feigned innocence then should drop each shape to freeze and adhere crystal and fine, would dispel all pretense.

Though soon once again, beneath dying lights we'll be followers to a cadence that pervades our own night through a once shapeless time, we'll forge discrete bounds and proclaim the new plans in synthetic sounds.

And then further on, a mass unapart past the charred, fallen trees, past all that would cling we will reach far with zeal and then with more cares to decipher arcane symbols, then describe all our prayers.

Abstract: This review serves as an introduction to the ideas of chemical topology as developed by the authors, drawing extensively on the pioneering work of the structural chemist-crystallographer Alexander F. Wells, who published the basic tenets of chemical topology during the mid-20th century. The reader is encouraged to further this study with a reading of the original literature on the subject, many of the topics discussed in here can be profitably followed up on by a perusal of one of the author's internet website at www.hexagonite.com for greater detail.

1. CHEMICAL TOPOLOGY

In this part, we describe the tenets of chemical topology and certain rational approximations to the transcendental mathematical constants ϕ, e and π that arise out of considerations of both: 1. the Euler relation for the division of the sphere into vertices, V, faces, F, and edges, E, and 2. its simple algebraic transformation into the so-called Schläfli relation, which is an equivalent mathematical statement for the polyhedra, in terms of parameters known as the polygonality, defined as $n = 2E/F$, and the connectivivty, defined as $p = 2E/V$. It is thus the transformation to the Schläfli relation from the Euler relation, in particular, that enables one to move from a simple heuristic mapping of the polyhedra in the space of V, F and E, into a corresponding heuristic mapping into Schläfli-space, the space circumscribed by the parameters of n and p. It is also true, that this latter transformation equation, the Schläfli relation, applies only directly to the polyhedra, again, with their corresponding Schläfli symbols (n, p), but as a bonus, there is a direct 1-to-1 mapping result for the polyhedra, that can be seen to also be extendable to the tessellations in 2-dimensions, and the networks in 3-dimensions, in terms of coordinates in a 2-dimensional Cartesian grid, represented as the Schläfli symbols (n, p), as discussed above, which do not involve rigorous solutions to the Schläfli relation. For while one could never identify the triplet set of integers (V, F, E) for the tessellations and networks, that would fit as a rational solution within the Euler relation, it is in fact possible for one to identify the corresponding values of the ordered pair (n, p) for any tessellation or network. The identification of the Schläfli symbol (n, p) for the tessellations and networks emerges from the formulation of its so-called Well's point symbol, through the proper translation of that Well's point symbol into an equivalent and unambiguous Schläfli symbol (n, p) for a given tessellation or network, as has been shown by Bucknum et al. previously. What we report in this communication, are the computations of some, certain Schläfli symbols (n, p) for the so-called Waserite (also called platinate, Pt_3O_4, a 3-, 4-connected cubic pattern), Moravia (A_3B_8, a 3-, 8-connected cubic pattern) and Kentuckia (ABC_2, a 4-, 6-, 8-connected tetragonal pattern) networks, and some topological descriptors of other relevant structures. It is thus seen, that the computations of the polygonality and connectivity indexes, n and p, that are found as a consequence of identifying the Schläfli symbols for these relatively simple networks, lead to simple and direct connections to certain rational approximations to the transcendental mathematical constants ϕ, e and π, that, to the author's knowledge, have not been identified previously.

1.1 Introduction

Bucknum [1] in work first described in 1997, outlined a general scheme for the systematic classification and mapping of the polyhedra, 2-dimensional tessellations and 3-dimensional networks in a self-consistent topological space for these structures. This general scheme begins with a consideration of the Euler relation [2] for the polyhedra, shown below as Eq. (1), which was first proposed in 1758 to the Russian Academy by Euler, and was, in fact, the point of departure for Euler into a new area of mathematics thereafter known explicitly as topology.

$$V - E + F = 2 \qquad \dots (1)$$

Relation (1) stipulates that for any of the innumerable polyhedra, the combination of the number of vertices, V, minus the number of edges, E, plus the number of faces, F, resulting from any such division of the sphere, will invariantly be that number 2, known as the Euler characteristic of the sphere. The variables known as V, E and F are topological properties of the polyhedra, or, in other words, they are invariants of the polyhedra under any kind of geometrical distortions. It is from this simple Eulerian relation, that we can develop a systematic and, indeed otherwise rigorous, mapping of the various, innumerable structures that present themselves, in levels of approximation, as models for the structure of the real material world within the domain of that area of science known as crystallography.

About a century after Euler's relation for the polyhedra was first proposed, as described above, the German mathematician Schläfli introduced a simple algebraic transformation of Euler's relation, for various purposes of understanding the relation better, and adopting it more effectively in proofs [3]. Thus, Schläfli introduced two new topological variables, like V, E and F before them, that were derived from them. Schläfli, therefore, defined the so-called "polygonality", hereafter represented by n, of a polyhedron as the averaged number of sides, or edges, circumscribing the faces of a polyhedron. He conveniently defined such a polygonality, as n = 2E/F, where, in this instance one can see that because each edge E straddles two faces, F, the definition is rigorous. Similarly, Schläfli introduced the topological parameter called the "connectivity", hereafter represented by p, of a polyhedron as the averaged number of sides, or edges, terminating at each vertex of a polyhedron. He conveniently defined such a connectivity, as p = 2E/V, where, in this instance one can see that because each edge E terminates at two vertices, V, the definition is rigorous.

From these definitions of n and p as topological parameters of the polyhedra, Schläfli was able to show quite straightforwardly, by algebraic substitution, that a further relation exists among the polyhedra in terms of their Schläfli symbols (n, p) [3]. It is from this equation, the Schläfli relation, shown as Eq. (2) below, that one can see that not only do the polyhedra rigorously obey 2, but it is also true that their indices as (n, p), that serve as solutions to 2, in addition lead to a convenient 2-dimensional grid, or Schläfli space, over which the various polyhedra can be unambiguously mapped, as has been explained by Wells in his important 1977 monograph on the subject [4].

$$\frac{1}{n} - \frac{1}{2} + \frac{1}{p} = \frac{1}{E} \qquad \dots (2)$$

Figure 1 due to Wells [4], below, illustrates the application of this type of Schläfli mapping for the regular Platonic polyhedra, where one sees that the point that belongs to the origin of this mapping, is indeed given by the Schläfli symbol (n, p) = (3, 3). The symbol (3, 3) represents the Platonic solid known as the tetrahedron, or by the symbol "t" in the map, known since Antiquity by the Greeks. Thus, as it is cast as the origin of this mapping of polyhedra, it is apparently, the only self-dual polyhedron. Similarly (4, 3) is the Platonic solid of the Greeks known as the cube, or "c" in the map, (5, 3) is the Platonic solid of the Greeks known as the dodecahedron, or "d" in the map, (3, 4) is the Platonic solid of the Greeks known as the octahedron, or “o” in the map, and (3, 5) is the Platonic solid of the Greeks known as the icosahedron, or “i” in the map.

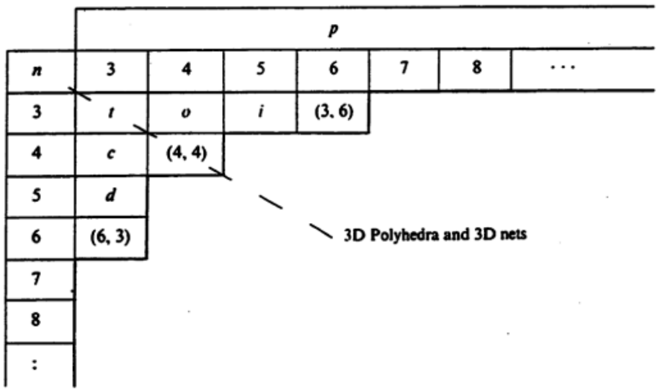

Fig. 1: Topology Mapping of the Platonic Polyhedra Due to Wells

Although the mapping of the Platonic polyhedra, shown in Fig. 1, indeed involves only those polyhedra in which the ordered pairs (n, p) are integers, it is readily transparent that one could magnify the map to include those polyhedra in which the polygonality “n” is fractional, these are the so-called Archimedean polyhedra, discovered by Archimedes in Ancient Greece [5]. In addition, the map could be magnified to include those polyhedra in which the connectivity “p” is fractional, these are the so-called Catalan polyhedra, discovered in Europe in the 19th century [6]. And finally, the so-called Wellean polyhedra [7], discovered in the 21st century [8], in which both indexes, “n” and “p”, are fractional, could be mapped in this Schläfli space of the polyhedra, without any loss of mathematical rigor.

1.2 Mapping of Tessellations and Networks

Wells also suggested [4], that the tessellations, which are structures or tilings extended into 2-dimensions and filling the plane, could have nominal labels attached to them, in the form of the Schläfli symbols (n, p), that, while not leading to rational solutions of the Schläfli relation, were, still it seems, rigorously defined from inspection of the topology of these elementary tessellations. Thus in order to extend the mapping in Schläfli space, the space of (n, p), some loss of rigor with regard to the Schläfli relation for the polyhedra had to be introduced, when considering the patterns known as tessellations. Wells, therefore included, explicity, the mapping of the square grid, given by the Schläfli symbol (4, 4), and the honeycomb grid, given by (6, 3), as well as the closest-packed tessellation, given by (3, 6), in his topology mapping, shown in Fig. 1, along with the Platonic polyhedra. He thereby extended the mapping to the tessellations, and later he implied that such a mapping could be extended to include the 3-dimensional (3D) networks as well, with a concomitant further loss of mathematical rigor, in that the values assigned as (n, p) to the various tessellations and networks were not rigorous solutions to Eq. (2).

It is also true that Wells [7], perfectly well introduced a systematic and rigorous coding of the topology of tessellations and networks he worked with, which is now called the Wells point symbol notation, and that this was a simple coding scheme over the circuitry and valences, about the vertices, in the unit of pattern of the tessellations and networks. The Wells point symbol notation was, however, nonetheless an important development for the rigorous mathematical basis it put the tessellations and networks on, formally, as quasi-solutions (n, p) for the Schläfli relation shown as Eq. (2).

Therefore, in a generic case of the Wells point symbol notation, one could have such a symbol for an a-, b-connected, binary network, given as $(A^a)_X$ $(B^b)_Y$, such that the exponents “a” and “b” nominally represent the valences of the 2 vertices in the tessellation or network of interest, and the bases “A” and “B” give the respective relative polygon sizes (circuit sizes) in the tessellation or network, while the parameters “X” and “Y” describe the binary stoichiometry of the network. In this generic case, we see that “X/Y” represents the number of structural components, identified by their topology character as (A^a), to the number of structural components identified by their respective topology as (B^b), that occur in this characteristic ratio in the structure, as specified by the unit of pattern.

Despite his invention of this elegant notation, Wells, for some odd reason, never explicitly showed how to translate the language of the Wells point symbol $(A^a)_X$ $(B^b)_Y$, rigorously into a Schläfli symbol (n, p), as was later shown elsewhere. Thus Bucknum et al., in 2004 [9], showed that the translation of the Wells point symbol into an, otherwise, from the perspective of Eq. (2), rigorous set of values (n, p) for the purpose of mapping tessellations and networks, was achievable if one used the following straightforward, simple formulas (applicable in this case for a generic Wellsean, binary stoichiometry structure) for the ordered pair (n, p), which can later be employed in the mapping of the structure, as is shown by Eqs (3).

$$n = (a \cdot A \cdot X + b \cdot B \cdot Y)/(a \cdot X + b \cdot Y) \qquad \text{... (3a)}$$

$$p = (a \cdot X + b \cdot Y)/(X + Y) \qquad \text{... (3b)}$$

It should, of course, be noted that one has to proceed with care in using Eqs (3a and 3b), in this topology analysis of structures, by carefully normalizing the circuitry traced around the p-connected vertices of the structure (paying careful attention to the parameters "a" and "b" above), by rigorously translating the circuitry of a given structure, into a vertex connectivity for the network of interest, by employing a vertex translation table like that shown below.

Table 1: Vertex Connectivity, p, as a Function of Circuit Number

Name	Vertex connectivity	Circuit number
Trigonal planar	3	3
Square planar	4	4
Tetrahedral	4	6
Trigonal bipyramidal	5	9
Square pyramidal	5	10
Octahedral	6	12
Cube centered	8	24
Anti-cube centered	8	28
Closest packed	12	60

Therefore, from the use of Eqs (3), for a binary stoichiometry, Wellsean net with topology $(Aa)_X (B^b)_Y$, or some other homologous translation formulas, as shown, for example, by Bucknum et al. for various elementary structural cases [9], it becomes, evidently, rigorously possible to precisely map the topology of any structure, including of course the polyhedra, but extendable to the vast body of the known tessellations and networks, that have been discovered and characterized crystallographically, otherwise by their symmetry character, now by their topological character in the form of a mapping in an extended Schläfli space, as is shown in Fig. 2 below.

n \ p	3	4	5	6	7	8	...
3	t	o	i	(3,6)	(3,7)	(3,8)	
4	c	(4,4)	(4,5)	(4,6)	(4,7)	(4,8)	
5	d	(5,4)	(5,5)	(5,6)	(5,7)	(5,8)	
6	(6,3)	(6,4)	(6,5)	(6,6)	(6,7)	(6,8)	
7	(7,3)	(7,4)	(7,5)	(7,6)	(7,7)	(7,8)	
8	(8,3)	(8,4)	(8,5)	(8,6)	(8,7)	(8,8)	
⋮							

Fig. 2: Extended Schläfli Space of the Platonic Structures

1.3 A Survey of the Topology of Structures

As Eqs (1) and (2), and Figs 1 and 2 explicitly reveal, it is the Platonic solids that form the basis of this mapping formulation of structures described in this paper. These forms, as shown in Fig. 3 with their appropriate polyhedral face symbolism [10], as discovered in Ancient Greece from the application of pure thought, were implicated later on in Plato's Timaeus, as the building blocks of Nature [11]. With the advent of modern crystallographic techniques by the Bragg's in the 20th century [12], we have come to learn that the structure of matter does indeed often take on various vestiges of these eternal objects. And so they have come to be important in modern structural chemistry as elucidated by Pauling [13] and others.

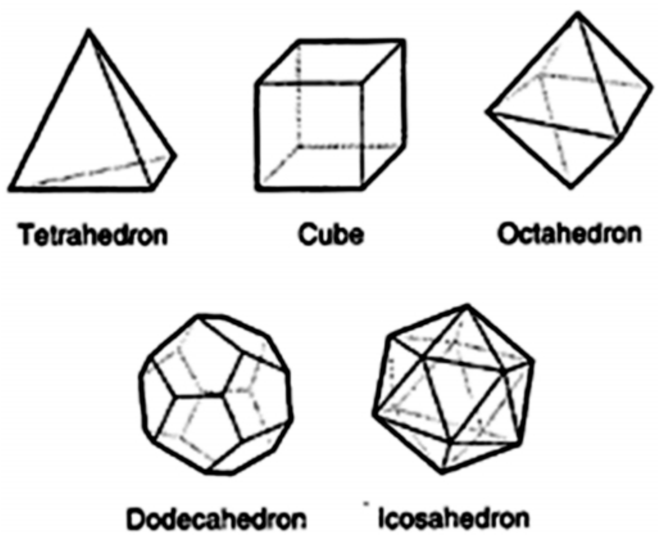

Fig. 3: The Platonic Polyhedra, with their Corresponding Polyhedral Face Symbols and Wells Point Symbols, Comprised of the Tetrahedron (3^4 and 3^3), the Octahedron (38 and 34), the Icosahedron (3^{20} and 3^5), the Cube (4^6 and 4^3), and the Dodecahedron (5^{12} and 5^3)

The polyhedra, thus forming the basis of the topology map of structures in Fig. 2, and also rigorously obeying the topology relations shown as Eqs (1) and (2) above, are positioned uniquely in this construction to support the vast space of tessellations and networks that, as we have seen in the preceding Section, can be mapped, rigorously, in Fig. 2 by the identification and proper translation of their Well's point symbols, as described above, into ordered pairs as Schläfli symbols (n, p). Plato's great work, Timaeus, thus predicted the ascendancy of the material world into perfect forms, in which the Platonic polyhedra hold primacy and support the overall organizational structure of matter, from which the innumerable other polyhedral objects, and the innumerable 2 D tessellations, and the innumerable 3 D networks, together all emerge as perfect objects, in this scheme.

Later, it has been shown by Duchowicz et al. [14], that indeed molecular structures can be represented in the scheme of Fig. 2, and they have a corresponding set of two topology relations (in addition to $n = 2E/F$ and $p = 2E/V$), shown as Eqs (4) and (5) below, that govern their mapping into Fig. 2.

$$V - E + F = 1 \qquad \text{... (4)}$$

$$\frac{1}{n} - \frac{1}{2} + \frac{1}{p} = \frac{1}{2E} \qquad \text{... (5)}$$

In this way, one can see that the overall chemical topology scheme described here, is a complete description of the topology of all matter constituting the material world. This communication will not treat the specific applications of Eqs (4) and (5), but it will be left to the reader to refer to those applications suggested in the literature [14].

Moving from the polyhedra and molecular fragments, as described above, one can then map the regular tessellations as shown in Fig. 4, with the honeycomb tessellation, given by the Wells point symbol notation as 6^3, and translated into the mapping symbol or Schläfli symbol as (n, p) = (6, 3), and the square grid, given by the Wells point symbol notation as 4^4, and translated into the mapping symbol or Schläfli symbol as (n, p) = (4, 4), and finally, the third regular tessellation, which thus outlines the space of Fig. 2 in terms of the tessellations, as the closest-packed grid, given by the Wells point symbol notation as 3^6, and translated into the mapping symbol or Schläfli symbol as (n, p) = (3, 6).

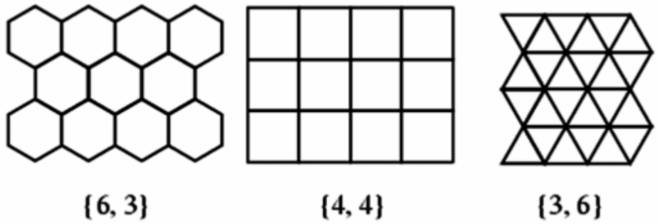

Fig. 4: The Platonic Tessellations, with their Corresponding Wells Point Symbols, Given as the Closest-packed Grid (3^6), the Square Grid (4^4) and the Honeycomb Grid (6^3)

One can, of course, insert all manner of hybrid tessellations, among these 3 regular ones, and generate innumerable Archimedean, Catalan and Wellsean tessellations. Some hybrid tessellations of the square grid-honeycomb grid pair have been analyzed topologically by Bucknum et al. [15]. There are, of course, an infinity of such structural tessellations, and they indeed fill the space in the neighborhood of the borderline between the polyhedra and the tessellations, on the one hand, and the tessellations and the networks in 3D, on the other hand. It is also true that Wells and others [4], have identified tessellations of the plane comprised of 5-gons and 7-gons, and their have been tessellations of 4-gons and 6-gons that admit unstrained 8-gons, and there are many more tessellations proposed, some of which have been taken as models of various C allotropes [16–18], which essentially can possess any n-gons in their pattern, provided that the restraint of being regular n-gons is relaxed. And it is thus true, that all of this infinity of tessellations can be mapped, rigorously, by the methods outlined above.

Finally, the map in Fig. 2 outlines the 3D networks, and a prominent member is, of course, the diamond lattice given by the Wells point symbol 6^6, which is translated [9] into the Schläfli symbol (6, 4). By examination of Fig. 2, one can see that the diamond network, given the Schläfli symbol (6, 4), is situated just across the borderline from the 2-dimensional honeycomb tessellation given by (6, 3) in the map. One member of the diamond network topology, is in a cubic symmetry space group of Fd-3m, space group #227, one of the highest symmetry space group patterns. There are, in fact, innumerable possible polytypic patterns within the diamond topology, several of these have been discussed recently by Wen et al. [19] in some detail, and all of them collectively possess the same Wells point symbol of 66, and the corresponding Schläfli symbol of (6, 4). It is only by their symmetry character, that the members of the diamond polytypic series can be distinguished from each other. Thus, the simplest cubic diamond polytype, known as 3C, is shown in Fig. 5 below.

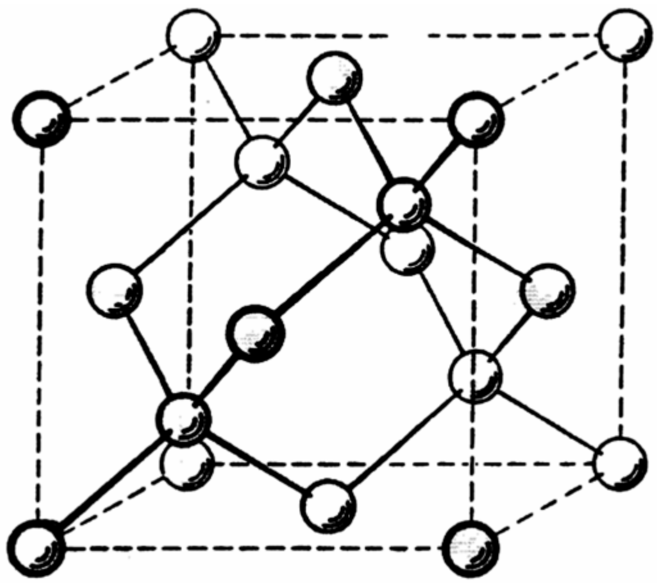

Fig. 5: Cubic Diamond (3C) Polytype, with the Wells Point Symbol (6^6), Lying in Symmetry Space Group (Fd-3m)

Thus in the diamond network, which corresponds to the Platonic (integer) topology of the Platonic polyhedra, one can readily trace the uniform 6-gon, puckered circuitry of the network connected together by all 4-connected, tetrahedral vertices. Diamond's topology classifies the network as a regular, Platonic structure-type.

Next, we move to the space between (6, 3) and (6, 4), seemingly between 2D and 3D forms, and investigate what potential structures might emerge along this boundary area. Such an examination turns up two distinct families of Catalan networks, that together possess the Catalan Wells point symbol $(6^6)_x$ $(6^3)_y$. One can see, through this Wells point symbol notation, that we are describing hybrid structures of the honeycomb tessellation, the so-called graphene grid, 6^3, and the diamond network, 6^6. The notation "y/x" specifies the stoichiometry of the net, in terms of the ratio of 3-connected, trigonal planar vertices, to 4-connected, tetrahedral vertices in the hybrid structure [20].

Thus one example of such a class of hybrid "graphene-diamond" structures is shown in Fig. 6, and these forms are known, by their hybrid topology, as the "graphite-diamond hybrids". They come in infinite series', in each of two varieties that are known as the ortho- form, and the para-form, these have been elegantly described by Balaban et al. in 1994 [21]. Collectively, as a family, they possess the Schläfli symbol of (6, $3^{(x/(x + y))}$), where the parameters "x" and "y" have the stoichiometric significance ascribed to them in the preceding paragraph. These structures, as a family, occupy the border-line area between (6, 3) and (6, 4) in the Schläfli map in Fig. 2.

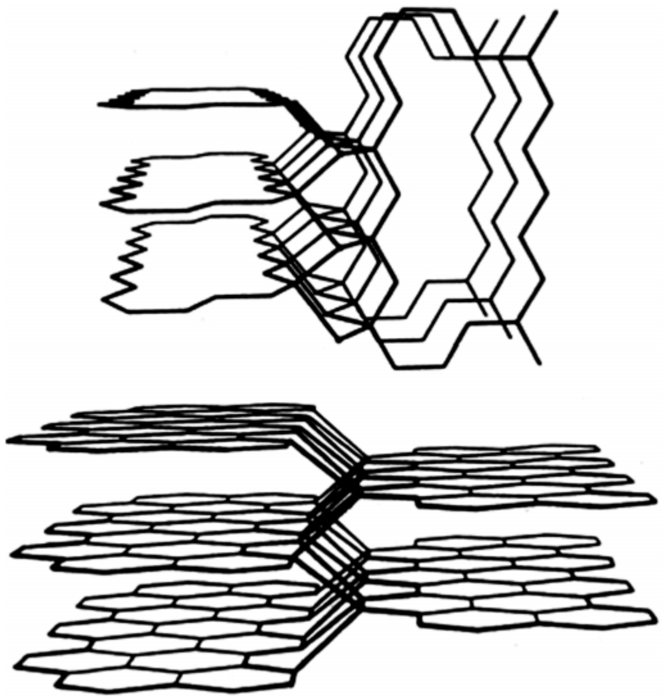

Fig. 6: Representatives of the Infinite Families of Ortho- and Para-graphite-diamond Hybrid Structures, with the Collective Wells Point Symbol $(6^6)_x$ $(6^3)_y$, of Orthorhombic Symmetry (Pmmm)

Yet another family of "graphite-diamond" hybrid structures to be considered, with the Wells point symbol $(6^6)_x$ $(6^3)_y$, and the corresponding Schläfli symbol given by (6, $3^{(x/(x + y))}$), is the family of structures described first by Karfunkel et al. [22] in 1992, as being built from the barrelene hydrocarbon molecular fragment, and extended by the insertion of benzene-like tiles to the parent framework, to generate many infinities of derived structures, which all, collectively, possess the hybrid graphite-diamond topology described above. Later, in 2001, Bucknum [23] clarified the details of the parent such structure derived by Karfunkel et al., and he called this structure "hexagonite" and the derived, such structures were known as the "expanded hexagonites". This name was assigned due to the symmetry space group of the parent structure, in P6/mmm, space group #191, and also due to the topology of the family of such structures, in which all circuitry over all members of the family, are comprised of 6-gons. The topological analysis of the hexagonite family, suggests that they begin with the Schläfli symbol (n, p) = (6, $3^{2/5}$), and extend from there, in descending, discrete increments of the connectivity, p, towards their termination at (n, p) = (6, 3), in the limit of the graphene grid topology. The parent "hexagonite" is shown in two views in Fig. 7.

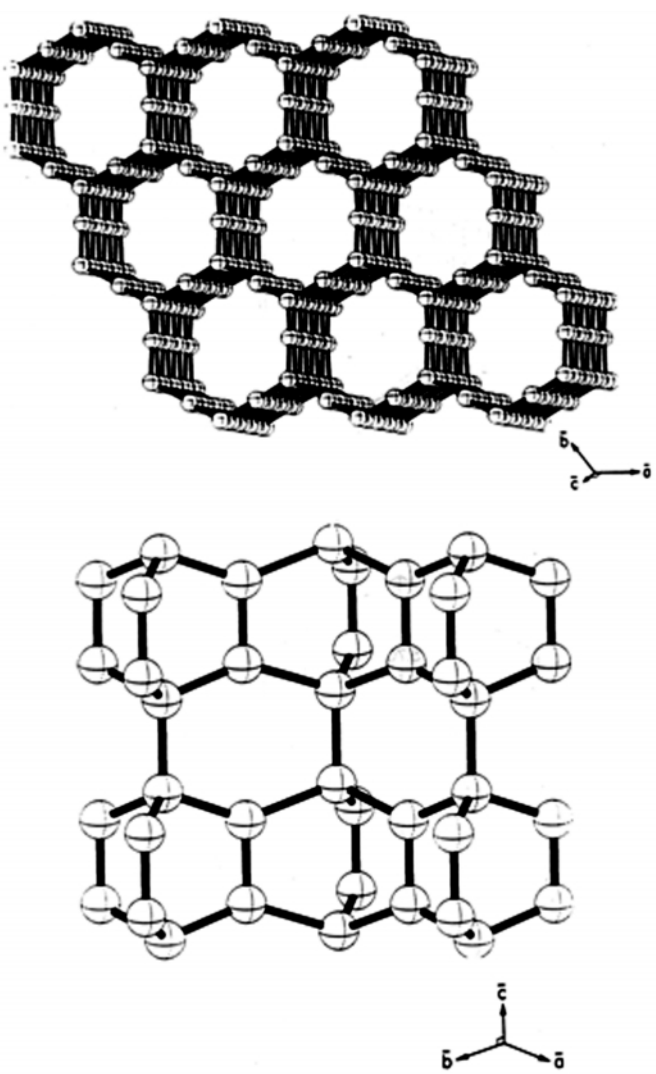

Fig. 7: Vertical and Lateral Views of Parent Hexagonite Structure of the Infinite Family of Hexgonites, with the Collective Wells Point Symbol $(6^6)_x\,(6^3)_y$, of Orthorhombic-trigonal-hexagonal (Pmmm, P3m1 and P6/mmm) Symmetries

It should be noted here that the so-called "graphite-diamond hybrids", as described above, are models for novel types of allotropes of carbon. In the vein of this discussion, it should be mentioned here that the border-line space in the topology map of Fig. 2, between the entry in the map of (5, 3), which is the pentagonal dodecahedron, and the entry in the map (6, 3) which is, of course, the graphene grid, lies the collective and infinite space of the fullerene C structures [24]. So, we can see that thus, the collective Schläfli symbol for the family of fullerenes is, in fact, given by ($5^{(x/(x+y))}$, 3), where, in this instance, "x" is the number of pentagons in the polyhedron, and "y" is the number of hexagons in the polyhedron [10]. The Schläfli symbol for the parent C allotrope called "Buckminsterfullerene" (C_{60}) is ($5^{5/8}$, 3) [24], and as substitution into Eq. (2) will show, this Schläfli symbol rigorously describes the Buckminsterfullerene polyhedron fully. Figure 8 shows a view of this polyhedron of icosahedral symmetry, and it is clear from this view that the polyhedron is uniformly 3-connected, (as the Schläfli symbol reveals, the fullerenes are Archimedean) and comprised entirely of 5-gon and 6-gon circuitry.

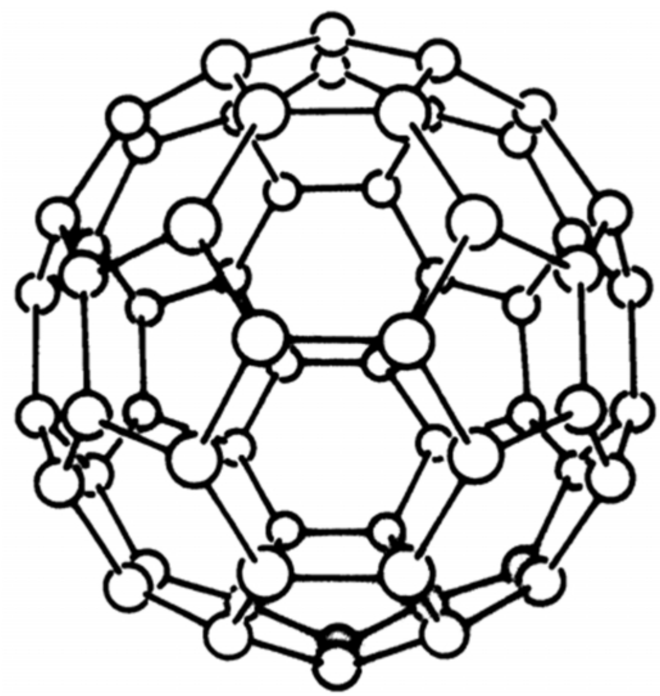

Fig. 8: The Parent Buckminsterfullerene Polyhedron, of the Infinite Family of Fullerenes, with the Collective Schläfli Symbol for the Family of Fullerenes given by ($5^{(x/(x+y))}$, 3), and the Fullerene Polyhedral Face Symbol of 5^x6^y, where "x" is the Number of Hexagons, and "y" is the Number of Pentagons, in the Fullerene, where Such Structures are of Icosahedral (Ih) and Lower Symmetry

Yet a final 3D network to be mentioned in this connection, which is a model of a 3-, 4-connected network of C, as opposed to a straight "graphite-diamond" hybrid, lying between (6, 3) and (6, 4) of Fig. 2, or a fullerene polyhedron, lying between (5, 3) and (6, 3) of Fig. 2, as in the preceding discussions with respect to allotropes of C; is the so-called "glitter" network of C invented by Bucknum et al. in 1994 [25]. This structure can be envisioned as being constructed from a 1, 4-cyclohexadiene building block, and it is shown in Fig. 9.

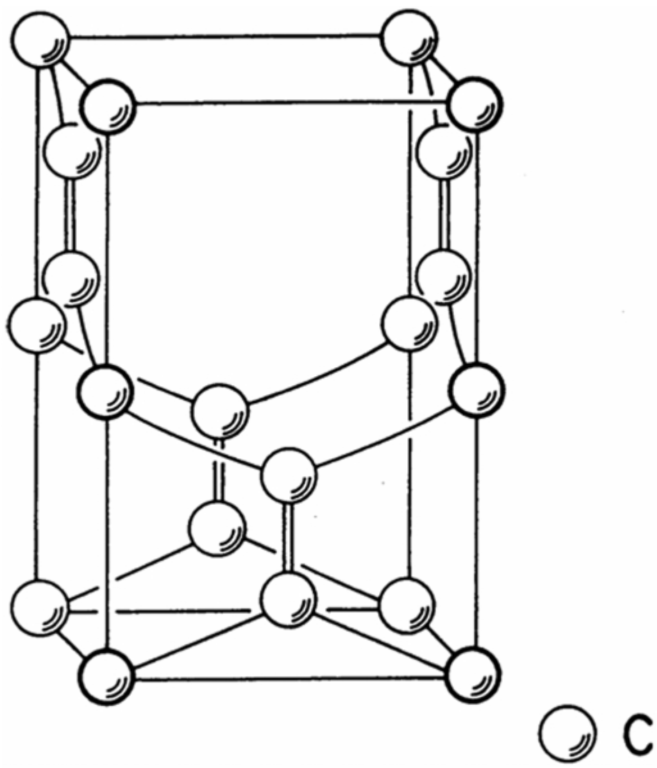

Fig. 9: Tetragonal Glitter Network of Carbon, with Wells Point Symbol given by $(6^2 8^4)$ $(6^2 8)_2$, and of Space Group Symmetry ($P4_2/mmc$)

As can be seen in Fig. 9, the Wells point symbol for this Wellsean network is given by $(6^2 8^4)$ $(6^2 8)_2$, and derived from this, is its Schläfli symbol of $(7, 3^{1/3})$ [9]. It is comprised of 6-gons admixed with 8-gons, in its topology, and an admixture of two trigonal vertices for every one tetrahedral vertex in its connection pattern. This particular C network has been important from the perspective of the 3-dimensional (3D) resonance structures which can be drawn over it, see Fig. 10, and there have been some favorable indications that its synthesis has been achieved [26-27].

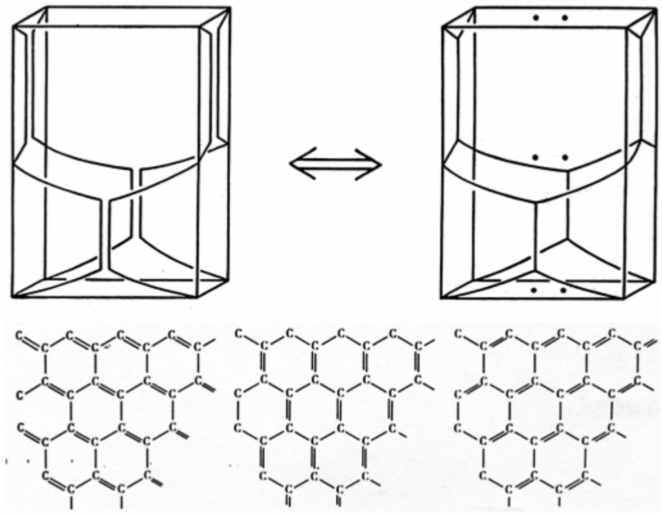

Fig. 10: Resonance Structures of the Graphite and Glitter Networks of C

Other inorganic networks that are of interest, that are not C allotropes, or models of C allotropes, would include the Archimedean Cooperite network, the structure of the minerals PtS and PdO [13], shown in Fig. 11, which is a 4-connected network comprised of an equal mixture of tetrahedral and square planar vertices, both of which are distorted in their geometries [22].

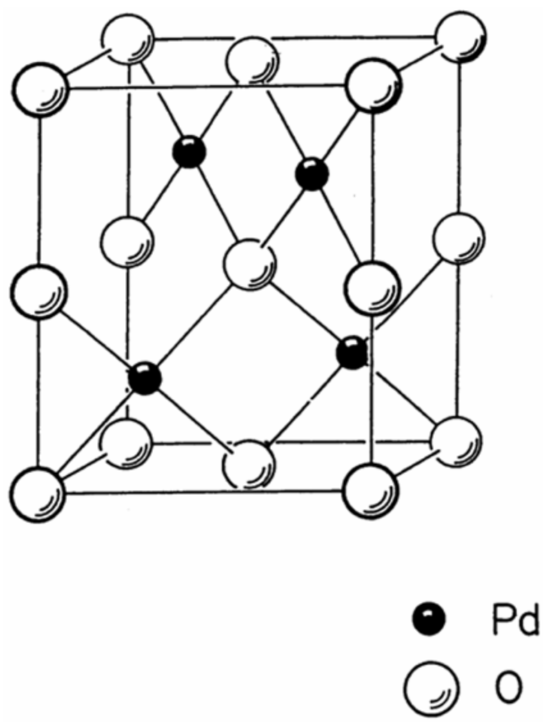

Fig. 11: Archimedean Cooperite Network as Structure of PdO and PtS, with the Wells Point Symbol of $(4^2 8^4)$ $(4^2 8^2)$, and of Space Group Symmetry ($P4_2/mmc$)

As Fig. 11 indicates, taking both tetrahedral and square planar vertices as equally 4-connected, one can thus assign an Archimedean topology to this network, with a Wells point symbol of $(4^2 8^4)(4^2 8^2)$, and a Schläfli symbol of $(6^{2/5}, 4)$ [9]. In this case, the network nominally is binary, with two distinct types of connectivity, and an apparently Wellsean topology associated with this, but, in fact in this instance, we have a 4-connected network where the square planar vertices (with 4 independent circuits) are viewed as equivalent in topology (if distorted) versions of the tetrahedral vertices (with 6 independent vertices).

Yet another inorganic network includes, but is not limited to, the Catalan fluorite network [13], the structure of a number of mineral fluorides including CaF_2, shown in Fig. 12.

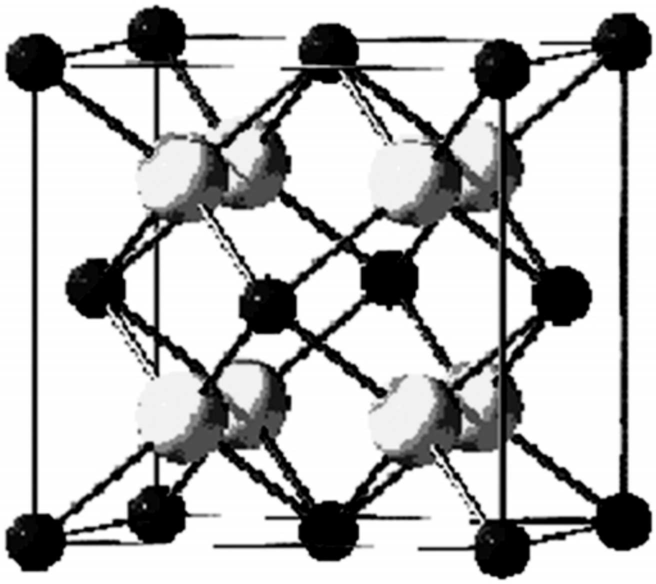

Fig. 12: Catalan Fluorite Structure as the Structure of CaF_2, this Network can be Represented by the Wells Point Symbol $(4^{24})(4^6)_2$, and Lies in Space Group (Fm-3m)

This densely connected network is comprised of 4-connected tetrahedral vertices, which are connected to each other through a uniform set of 4-gons. The topology of this network can be represented by the Wells point symbol (4^{24}) $(4^6)_2$, and this can be translated into a Catalan Schläfli symbol of $(4, 5^{1/3})$ [9]. It can be mapped in Fig. 2 just beyond the entry (4, 5).

Still another inorganic structure-type we can provide the topology of, is the rocksalt (or primitive cubic) lattice [13], which is the structure of a number of inorganic alkali metal halides and alkaline earth chalcogenides. The rocksalt lattice is shown in Fig. 13 below.

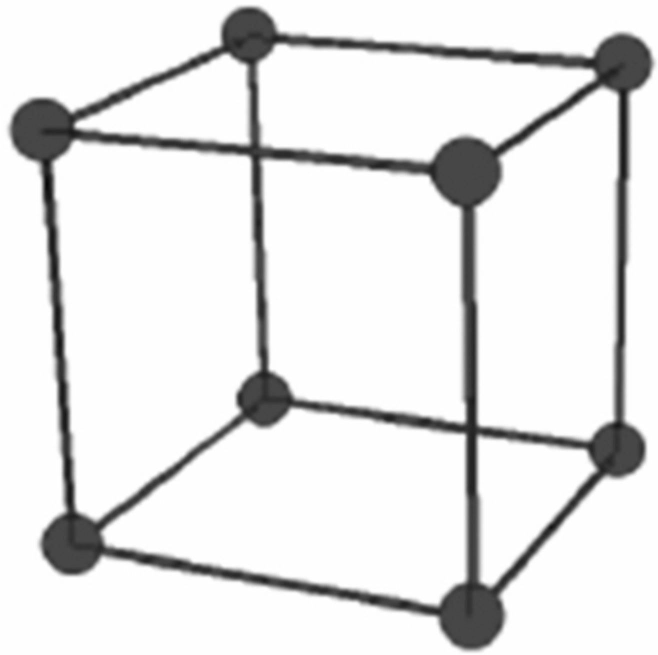

Fig. 13: Platonic Rocksalt Structure as the Structure of NaCl, this Network can be Represented by the Wells Point Symbol (4^{12}), and Lies in Space Group (Pm-3m)

Also known as the primitive cubic structure-type, the rocksalt lattice is comprised uniformly of octahedral 6-connection in all 4-gon circuitry. The Wells point symbol for the network is given as 4^{12}, and this can be translated into a Schläfli symbol for the network of (4, 6) [9]. Because this rocksalt network is of a Platonic (regular, integer) topology, it can readily be seen where it maps in Fig. 2. It represents, structurally, an extension into 3-dimensions (3D) of the square grid 44, or (4, 4) which extends in 2D, through a layering, in exact register, of other square grids onto a parent square grid, and their interconnection through perpendicular interlayer bonding through the respective vertices.

As a final inorganic structural-type that we can analyze here topologically in this Section, we have the so-called body-centered cubic (bcc) structure of CsCl [13], and a number of inorganic structures including alkali metal halides and alkaline earth chalcogenides and other materials. The bcc structure-type is shown here in Fig. 14.

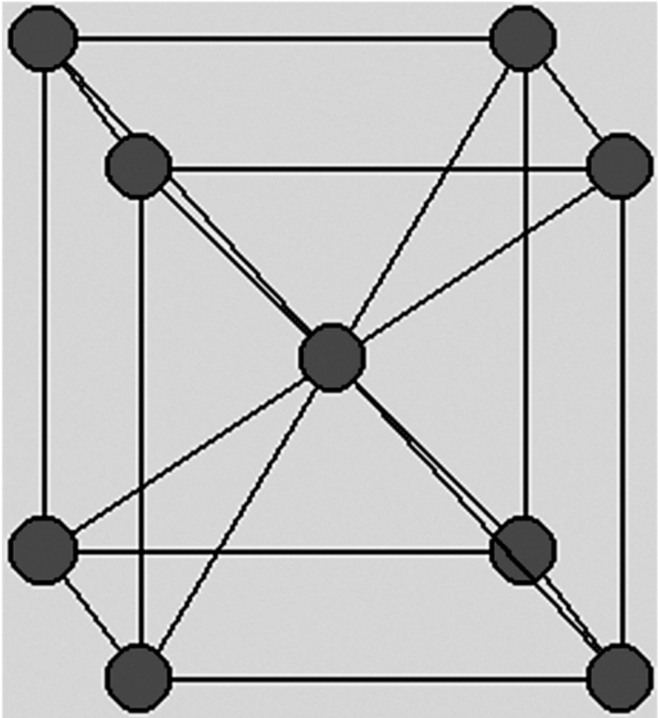

Fig. 14: Platonic Body-centered Cubic (b.c.c.) Structure as the Structure of CsCl, this Network can be Represented by the Wells Point Symbol (4^{24}), and Lies in Space Group (Im-3m)

It is uniformly comprised of 8-connected, cube-centered vertices that are mutually interconnected by all 4-gon circuits in the net. The topology of the bcc lattice can be specified by 4^{24}, or by the corresponding Platonic Schläfli symbol of (4, 8) [9].

There are, of course, innumerable other network structures that possess 3-dimensional geometries, one only has to look at the exhaustive works of O'Keeffe et al. to discern the scope of this field [28]. In the present discussion, we move, in the next Section, into the area of the topological analysis of some networks in 3-dimensions that exhibit rather odd Schläfli symbols (n, p). These networks, the oldest of which was identified only in 1951 (Waserite) [29], and the others of which were identified only in 1988 (Kentuckia) [30], and 2005 (Moravia) [31], suggest from the computation of their respective Schläfli symbols (n, p), by the methods outlined in Section 2 and Eq. (3) above, that such numbers represent not only topological parameters of these networks, but they coincidentally and fortuitously can be construed as rational approximations, in various instances, to the transcendental mathematical constants ϕ, e and π.

1.4 Rational Approximations to ϕ, e and π

Certain material networks, including the $CaCuO_2$ [30] (Kentuckia network [32]) structure-type, that is the progenitor for all of the superconducting cuprates, and the so-called Moravia structure-type [33], that is the proto-type structure for a number of coordination network (also called metal-organic frameworks or MOF's) structural compositions [31], and the so-called Waserite structure-type [29], that is the structure of the anionic, platinate sublattice of the ionic conducting lattice, known as sodium platinate ($NaPt_3O_4$), have here, through topological analysis, been shown, either to have a network polygonality, n, (Kentuckia network) the value of which serves as a rational approximation to the transcendental mathematical constant π, or, alternatively, they have a network connectivity, p, the value of which serves as a rational approximation to the product of the transcendental mathematical constants e and ϕ (Moravia network), or e and π (Waserite network).

The Kentuckia structure-type, proposed by Bucknum et al. in 2005 [32], is the pattern adopted by the high temperature superconducting cuprate composition, it is $CaCuO_2$ [30] that adopts this pattern, which is the progenitor to all the superconducting cuprates discovered so far. This tetragonal structure-type lies in space group P4/mmm, #123 and is shown in Fig. 15 below.

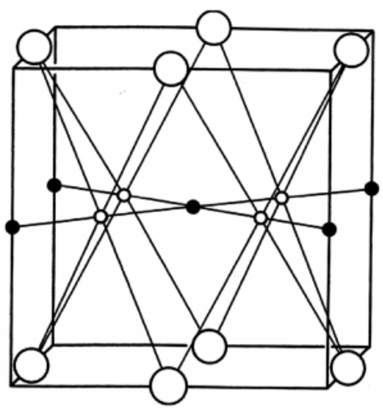

Fig. 15: Wellsean Kentuckia (ABC_2) Structure-type as the Structure of the Superconducting Cuprate Salt $CaCuO_2$, this Network can be Represented by the Wells Point Symbol (4^4) ($4^{12}6^{12}$) $(4^{12})_2$, and Lies in Space Group (P4/mmm)

It can be seen from Fig. 15 that this tetragonal oxide, bears a relation to the cubic perovskite ($BaTiO_3$, [13]) structure-type which lies in the cubic space group Im-3m, not shown here, in which, by removal of an axial pair of oxygen vertices, one can generate the Kentuckia structure-type from the perovskite structure-type. However, it should be pointed out that the perovskite structure-type is a 6-, 12-connected network, in which the transition metal titanium and chalcogenide oxygen centers, attain octahedral 6-coordination, while the alkaline earth barium cation bears a closest packed coordination sphere of 12. Whereas in the Kentuckia structure-type, the lattice, by great contrast as can be seen in Fig. 15, bears an oxygen vertex with a square planar, 4-connected coordination, and the transition metal copper vertex bears an octahedral, 6-connected coordination, while the alkaline earth calcium cation is in cube-centered, 8-fold coordination. It is a ternary, 4-, 6-, 8-connected tetragonal structural pattern, as is described in Fig. 15.

Thus the connectivity in Kentuckia, is that of a ternary 4-, 6-, 8-connected structural-type, while the connectivity in perovskite appears to be that of a binary 6-, 12-connected network topology. It appears that all the circuitry in perovskite is comprised of 4-gons with, perhaps, the stoichiometry AB4, in which the vertex “A” is in 12-connected, closest-packed topology, and the vertex “B” is 6-connected, octahedral coordination. This leads to a Wells point symbol for perovskite of $(4^{60})\ (4^{12})_4$ and a Schläfli symbol of (n, p) = (4, 7.2). Where, as a reference, the hexagonal closest packed (hcp) and cubic closest packed (ccp) networks, have the Wells point symbol 3^{60}, and a Schläfli symbol of (n, p) = (3, 12). In contrast, we see that the polygonality in the Kentuckia pattern, as revealed in Fig. 15, is a composite of 4-gons and 6-gons, with the Wells point symbol for the lattice being $(4^4)\ (4^{12}6^{12})\ (4^{12})_2$. As Eq. (6) reveals, the polygonality, n, for this structural-type, bears an odd resemblance to the transcendental mathematical constant, occurring as it does, within 1% of exactly the value of $\bullet 2\cdot\pi$.

$$n = (40\cdot 4 + 12\cdot 6)/52 \qquad \text{... (6a)}$$

$$n = \bullet 2\cdot\pi \qquad \text{... (6b)}$$

Turning to the Waserite network [29], which is shown to be a relatively simple, binary 3-, 4-connected network topology in Fig. 16.

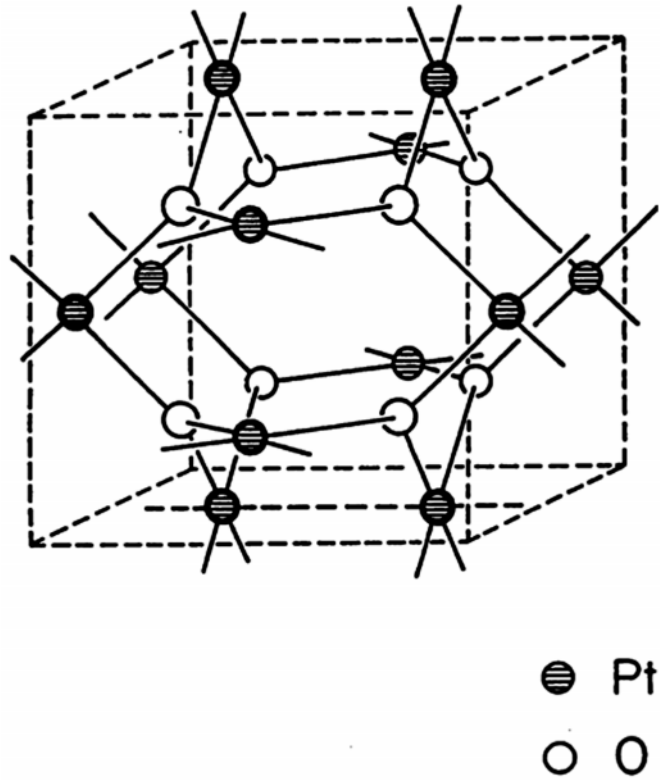

Fig. 16: Catalan Waserite Structure-type as the Structure of the Ionic Conducting Platinate Salt $NaPt_3O_4$ (Sodium Cations not Shown), this Network can be Represented by the Wells Point Symbol $(8^4)_3\ (8^3)_4$, and Lies in Space Group (Pm-3n)

As is revealed in Fig. 16, the 3-to-4 stoichiometry of 4-connected square planar vertices to 3-connected trigonal planar vertices, present in the Waserite topology, together with the Wells point symbol for this network as $(8^4)_3\ (8^3)_4$, thus demonstrates that this simple structure is indeed a binary, Catalan network comprised of all 8-gon circuitry. Therefore it is apparent, readily, that the polygonality is simply given by n = 8, in this pattern. But as has been described previously for this so-called Waserite network [34], the connectivity index of it, as shown in Eqs (7), suggests that its topology is more complex than meets the eye.

$$p = (3\cdot 4 + 4\cdot 3)/7 \qquad \text{... (7a)}$$

$$p = (2/5)e\cdot\pi \qquad \text{... (7b)}$$

As Eqs (7) reveals, it is a fact of simple arithmetic that the weighted average connectivity of the Waserite network, given by the symbol p, is in fact equal, to better than 99 parts in 100, to $(2/5)e\cdot\pi$. Here π is, the familiar ratio of a circle’s circumference to its diameter [35], and e is the natural base of exponentials [36]. These numbers are transcendental, as they are infinite, non-repeating fractions [35, 36]. An identical relation will also hold for the other structures patterned on a stoichiometry of four 3-connected vertices-to-three 4-connected vertices including, for example, the rhombic dodecahedron (given by the Catalan Wells point symbol as $(4^4)_6$ $(4^3)_8$), and the well-known phenacite network of Bragg et al. (not shown, given by the Wellsean ternary Wells point symbol (8^3) $(6^3)_3$ $(6^3 8^3)_3$ [37]).

Other relations emerging from such consideration of the connectivity index, p, in the Waserite structural-type include Eq. (8) [34], known hereafter as the Timaeus relation, for its suggestion of a Cosmogony based upon the 5 Platonic solids as enunciated by Plato [11].

$$(1)\cdot(2.3333333\ldots\ldots\ldots\ldots)\cdot e\cdot p = (4)\cdot(5) \quad \ldots (8)$$

Equation 8 suggests the ultimate simplicity of definitions of e and π, through an elementary relationship involving only the first 5 counting numbers, or alternatively, the first 4 prime numbers [34].

Finally, in this survey of crystalline structure-types which exhibit relations to the transcendental mathematical constants, in their structural topology, we turn to the so-called Moravia network [31, 33], first posited as a potential structural-type in 2005 by Bucknum et al. This Moravia network has, in fact, turned out to be the structure adopted by several coordination networks known as metal-organic-frameworks (MOF's) [31]. It is readily seen to be a Wellsean, 3-, 8-connected network upon careful inspection of the drawing for valences, and tracing of circuitry in Fig. 17.

The Wells point symbol for the Moravia structural-type is encoded as $(4^4 6^8 8^{12})_3$ $(4^3)_8$, it is thus a complex, Wellsean network composed of two connection motifs, the trigonal planar, 3-connected, and cube-centered, 8-connected, vertices, held together in circuits of 4-gon, 6-gon and 8-gon sizes. The complex Well's point symbol for the network, belies in this instance, the relatively high symmetry of the structure, in which Moravia is lying in the cubic space group Pm-3m, #221.

If we take the point symbol for the network, and analyze it according to Eqs (3) described above, the Well's point symbol translation formulas, one obtains the result that the weighted average polygonality for the network is indeed given by n = 6. The Waserite net is thus pseudo-Catalan, with

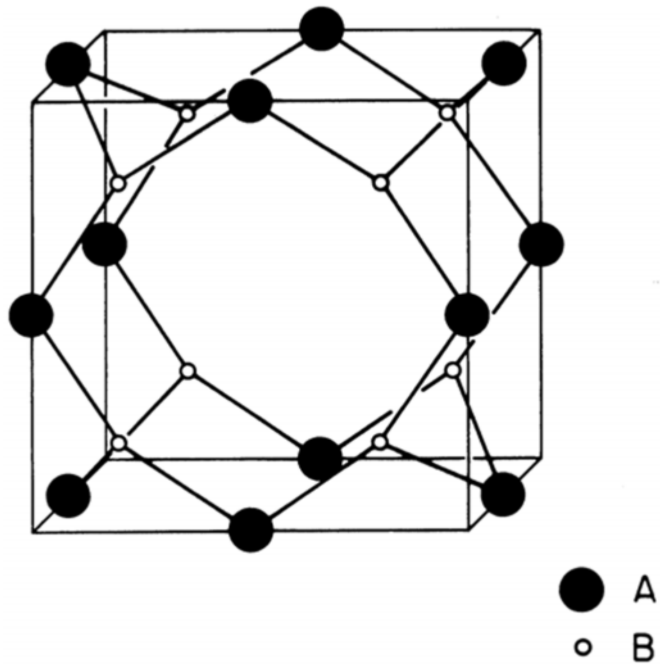

Fig. 17: Wellsean Moravia Structure-type as the Structure of Several Coordination Networks (Metal Organic Frameworks, MOF's), this Network can be Represented by the Wells Point Symbol $(4^4 6^8 8^{12})_3$ $(4^3)_8$, and Lies in Space Group (Pm-3m)

an integer polygonality of 6, that is nonetheless the result of averaging over 4-, 6- and 8-gons in its structural pattern. Upon calculating the connectivity index, p, for Moravia, however, we get the result shown in Eq. (9).

$$p = (3\cdot 8 + 8\cdot 3)/11 \quad \ldots (9a)$$

$$p = e\cdot\phi \quad \ldots (9b)$$

Thus it is seen that the connectivity index, p, of Moravia, as a 3-, 8-connected network, is equivalent, to better than 99 parts in 100, to the product of the two transcendental mathematical constants ϕ [38] and e [36], given simply as $\phi\cdot e$. Here, as above, e is the natural base of exponentials [36], and ϕ is the well-known golden ratio [38], as is expressed in Eq. (10).

$$\phi = (\sqrt{5} + 1)/2 \quad \ldots (10)$$

Equations (9), like the transformation of Eqs (7) to (8) above, can be factored, interestingly, so that the relation of $\phi\cdot e$ evolving out of the topology of the Moravia structure, as shown in Fig. 17 above, involves the first 6 Fibonacci numbers, F (1-to-6) (given, on the left, in Eq. (11b) as 1, 1, 2, 3, 5, and 8), and these are related to the 10th Fibonacci number, F (10) (given, on the right, in Eq. (11b) as 55).

$$F(1)\cdot F(2)\cdot F(3)\cdot F(4)\cdot F(5)\cdot F(6) = (e)\cdot(\phi)\cdot F(10) \quad \text{... (11a)}$$

$$(1)\cdot(1)\cdot(2)\cdot(3)\cdot(5)\cdot(8) = (e)\cdot(\phi)\cdot(55) \quad \text{... (11b)}$$

These relations between the topology of these structures in this Section, as is revealed by the computation and mapping of their corresponding Schläfli symbols (n, p), and the transcendental mathematical constants ϕ, e and π, that can be thus correlated to their structural character, suggest the mathematical, and potentially scientific, richness that such structures may lead to.

1.5 Overview on Chemical Topology

In this paper we have reviewed the basic tenets of a chemical topology scheme, one that can be applied to classify and effectively map the innumerable polyhedra, tessellations and networks, based upon a simple computation of their Schläfli symbols (n, p), from translation of their corresponding Wells point symbols. A restriction pointed up by this work, is that all structures in such a chemical topology scheme must, indeed, be simply connected. The phrase "simply connected" means that all edges, E, in a structure, be it a polyhedron, tessellation or network, must terminate at distinct vertices, V, in the network, where such edges, E, are known as proper edges. A second condition on a net being "simply connected", is that all faces, F, in the structure should be bounded by proper edges, E, as defined in the preceding sentence. It is not clear, at this juncture, what form a systematic chemical topology would take on for the "non-simply connected" structures. As there are innumerable non-simply connected structures, to accompany the infinite number of simply connected structures in Schläfli space (the space of the Schläfli symbols (n, p)), it would seem that a topological analysis of these complex structures would be desirable and necessary to get a more complete handling of the chemical topology of crystal chemistry.

The brunt of this paper has been dedicated to a survey of some of the more prominent (well-known or obvious) organic and inorganic structure-types. Organic structures included some well-known C allotropes, like the regular, graphene grid and the regular, diamond network, both forms of C known since Antiquity. And, also, more modern C forms were surveyed, like the 3-, 4-connected, Catalan graphite-diamond hybrids [21], the 3-, 4-connected, Catalan hexagonite lattices [22, 23] and the Wellsean, 3-, 4-connected glitter C form [25], for which there is currently some evidences of their syntheses from the growth of C nanocrystals [26, 27]. Inorganic structures included in this survey, were the 4-, 8-connected, Catalan fluorite lattice, the 4-connected, Archimedean Cooperite lattice, the 8-connected, regular CsCl, body-centered cubic structure-type, and the 6-connected, regular rocksalt structure-type [13]. Finally, in this survey, lattices which admitted connections in their topology to the transcendental numbers included the 3-, 8-connected, Wellsean Moravia net, discovered in 2005 [31, 33] (related to ϕ and e, through the connectivity), the 4-, 6-, 8-connected, Wellsean Kentuckia (cuprate structure-type) net, discovered in 1988 [30, 32] (related to π, through the polygonality), and finally the 3-, 4-connected, Catalan Waserite net (platinate structure-type), discovered in 1951 [29].

The occurrence of relations to the transcendental numbers of mathematics, in the computations of the topology character of some of these networks, is indeed a mysterious outcome. It is not clear whether such relations could imply that the topology of these lattices, like the Kentuckia lattice, in which $n = \sqrt{2}\cdot\pi$, could indeed be equated to some type of ordering parameter for the lattice, such that by the introduction of systematic defects in the connectivity, p (or thereby the polygonality, n) over the bulk lattice, might lead to a corrected value of n, that asymptotically approaches the true value of π, and that, that might have some bearing on bulk properties of the Kentuckia network, like the critical superconducting transition temperature, T_c, in the cuprate composition $CaCuO_2$ [32]. Such considerations as these, open up new avenues of explorations for solid state scientists based upon the intrinsic topology character of such networks as these.

2. TOPOLOGICAL FORM

In this part, the topological form index, represented by I, is introduced and is defined as the ratio of the polygonality, n, to the connectivity, p, in a structure, it is given by I = 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, I, 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 I, 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 this part.

2.1 The Topological Form Index

During the 1950's A.F. Wells began his enumerative work on 2- and 3-dimensional networks and novel crystal structures [39]. 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 2- and 3-dimensional structural patterns (that is collections of vertices, edges and faces filling 2- and 3-dimensional 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 [39]. 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 [39], an augmentation of this map involved moving into frontier that included the various 2-dimensional 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 [25]. 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 1950's, 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 4 distinct structures that possessed the Schläfli symbol (7, 3) [39]. These 4 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) [39]. 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 [7].

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 [25], is defined as the ratio of the polygonality to the connectivity in a given structure, I. This is shown in Eq. (12) [1]:

$$I = n/p \qquad \text{... (12)}$$

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.

2.2 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 [40], 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 Eq. (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 [2]. Euler envisioned the inscription of the polyhedra inside the sphere, in order to establish the relation shown in Eq. (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 [40].

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 2 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, I, 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, I. For if corresponding structures between the polyhedral class and the class of 2D tessellations possess the same topological form index, I, 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 [40], 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 [39]. 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 Eq. (13), holds:

$$\text{area }(3, 3) = \text{area }(4, 4) = 2/\sqrt{3} \qquad \ldots (13)$$

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 [39]. 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 [40]. 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:

$$\frac{\text{area}_{(4,3)}}{\text{area}_{(4,4)}} = \frac{\text{area}_{(4,4)}}{\text{area}_{(4,6)}} \qquad \ldots (14)$$

By substitution the unknown in 14, area (4, 6), can be solved for as is shown in Eq. (15).

$$\text{area}_{(4,6)} = \text{area}_{(4,4)}\left(\frac{\text{area}_{(4,4)}}{\text{area}_{(4,3)}}\right) = \text{unity} \qquad \ldots (15)$$

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.

2.3 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) [25] 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, I, of Eq. (5), and the corresponding elementary polygonal circuit area, labeled area (n, p).

Table 2 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) [41], the diamond structure-type labeled as (6, 4) [13] and the (primitive cubic net) rocksalt structure-type labeled as (4, 6) [39] are the regular structures, and they possess ideal bond angles. The Cooperite structure-type labeled as $(6^{2/5}, 4)$ [42] 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) [29] is Catalan and has ideal bond angles, and the glitter structure-type with the Schläfli index (7, 31/3) [25] is topologically irregular and has ideal tetrahedral angles and distorted trigonal planar angles assumed in the calculation of its polygonal circuit area.

Table 2
Geometrical-Topological Data for 12 Structures

Name	(n, p)	I = n/p	Area (n, p)
cp 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)	$1^{1/2}$	$\sqrt{2/3}\cdot$•
Cooperite (PtS)	$(6^{2/5}, 4)$	$1^{3/5}$	$2\sqrt{2}\pi/3$
honeycomb net	(6, 3)	2	3
glitter	$(7, 3^{1/3})$	$2\pi/3$	$\sqrt{2/\sqrt{3}}\cdot$•
Waserite (Pt_3O_4)	(8, (2/5)e·•)	$2^{1/3}$	•2·e
$ThSi_2$	(10, 3)	$3^{1/3}$	7•3/2

One can see immediately that the form indexes, I, 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. The diamond structure-type given by (6, 4) and illustrated elsewhere [13], with unity edge length and tetrahedral bond angles, has an elementary polygonal face area of exactly $\sqrt{2/3}\cdot\pi$. The Waserite structure-type given by (8, 3.4285) and illustrated and discussed previously [29], a Catalan network in 3D, has octagonal elementary polygonal circuits in its structure which have exactly the face area of $\sqrt{2}\cdot e$ 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 [25], has a form index, I, of $2\pi/3$, 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, it is given as $\sqrt{2/\sqrt{3}}\cdot\pi$.

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 [40]. The Wells coincidences suggest that the polygonal circuit area of the chair hexagons in the diamond lattice [13], for instance, is just a scaling of π. They suggest that the area of the 8-sided circuitry in the real Waserite phase [29], 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 1000's in terms of those observed as pure forms in models of various polyhedra and 2D and 3D structural-types [39], 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 $\sqrt{2/3}\cdot\pi$, for example. It must not be overlooked in this context that with the 3 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.

2.4. The Wells Conjecture and Geometrical-Topological Correlation

Data from Table 2 has been mapped to a graph in which the topological form index, I, 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 Fig. 18. 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 I. 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:

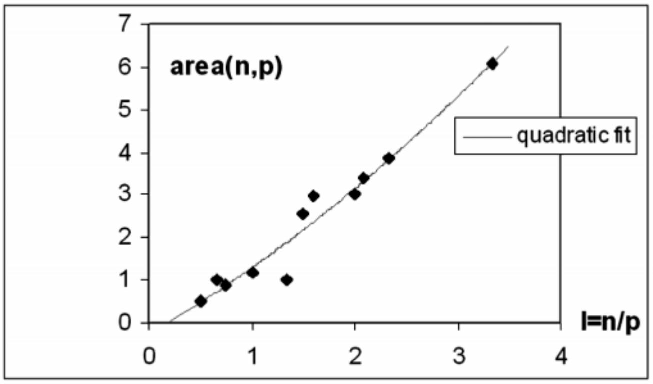

Fig. 18: Regression Fit of the Data in Table 1 Representing the Elementary Polygonal Circuit Area, Area (n, p), Versus the Topological form, 1, for the 12 Structures

$$\text{area}\,(n, p) = A\cdot I^2 + B\cdot I + C \qquad \text{... (16)}$$

The parameters in Eq. (16) 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 Eq. (16) from corresponding sets of 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, I, for structures and their elementary polygonal circuit area, area (n, p), suggests a mathematical conjecture which is called the Wells conjecture [40]. 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 I, 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 Eqs (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.

2.5 Overview of Topological Form

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, I, 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 I correlates with density, in fact empirical evidence from hexagonite and the expanded hexagonites [23] suggests strongly that I is not a measure of density. It is suggested here that the term compactness be used with reference to I, 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 I correlates with low elementary polygonal circuit area and high compactness, and vice versa.

It is important to point out the significance of Eq. (9) in terms of the space of all possible networks [39]. Equation (16) represents a set of points through the space of all possible networks (all potential values of the parameter I = n/p). It thus identifies those networks with a given set of coordinates in the space (I, 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 [9]. From the associated topological symbol (n, p) computed in this way, one can use Eqs (12) and (16) in this paper, to calculate the corresponding values of such a structure given by the topological form index, I, and the area of the elementary polygonal circuit, area (n, p), respectively.

By plotting the coordinates in this manner as given for example by Fig. 1 for the set of 12 structures, one could therefore locate that point in the space represented by the graph of Eq. (16). If in fact such a point doesn't fall in the proximity of the curve given by Eq. (16), 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 Eq. (16) 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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It Appears that the 5 Platonic Polyhedra Obey Eq. (2) of the Text, if one Specifies their Topology by a Well's Point Symbol, Given by Aa, in which n = A and p = a, and there is no Relation between this Well's Point Symbol, Aa, and the Computation of V, E and F in the Euler Model of Eq. (1). It is Also the Case, that the 5 Platonic Polyhedra Obey Eq. (2) of the Text, if one Specifies their Topology by a Polyhedral Face Symbol, Given as Ab, in which (b · A) = 2E, b = F, and V is Defined through the Euler Relation for the Sphere, and then n = 2E/F and p = 2E/V, by Definition.

For the Archimedean Polyhedra it Appears that it is Only Possible to Specify (n, p), for Insertion into Eq. (2), by Encoding a Polyhedral Face Symbol, Given as AaBbCc……., where a is the Number of A-gons, in a Ratio with b B-gons, etc. for the Polyhedron, and thus, in which (a · A + b · B + c · C + …….) = 2E, (a + b + c + ……) = F, and V is Defined through the Euler Relation for the Sphere, and where Finally then, n = 2E/F and p = 2E/V, by Definition. While for the Catalan and Wellsean Polyhedra, by Contrast, it Appears that it is Only Possible to Specify (n, p), for Insertion into Eq. (2), by Encoding a Wells Point Symbol, given as $(A^a)_x (A^b)_y (A^c)_z$………., where a is the Number of A-gons Meeting at a, and b is the Number of A-gons Meeting at b, etc. and x, y, z, etc. Specify the Stoichiometry of the Polyhedron, for the Catalan or Wellsean Polyhedron of Interest, in which (a · A + b · A + c · A + ……..) = E, (a · x + b · y + c · z + ………) = 4F and (x + y + z + ……..) = V, where Finally then, n = 2E/F and p = 2E/V by Definition, as Throughout.

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The Wells Fundamental Polyhedra Metric, the Wells Structural Correspondence Principle and the Wells Morphological Principle, all 3 used in this Paper to Derive the Polyhedral and 2D and 3D Metrics, and to Determine the Data in Table 1; and the Wells Coincidences and the Wells Conjecture, which Emerge as a Consequence of the Data in Table 1; have been Collectively Named to Honor Professor A.F. Wells who was at the University of Connecticut, Storrs for Some Years, where he Established Himself as a Master of Applied Topology and Derived more than 100 Novel Networks.

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