MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **54** (2005) 89-119

ISSN 0340 - 6253

Calculating Topological Indices of Networks from the Corresponding Wells Point Symbol

Michael J. Bucknum
Georgia College & State University, Department of Chemistry and Physics, CBX 82, Milledgeville, GA 31061, U.S.A.

Eduardo A. Castro*
INIFTA, Theoretical Chemistry Division, Chemistry Department, Faculty of Exact Sciences, Suc.4, C.C. 16, La Plata 1900, Argentina

(Received September 20, 2004)

Abstract-This paper begins with a review of the Euler relation for the convex polyhedra. The Schläfli relation is derived from this by introducing the secondary topological indices of polygonality and connectivity. A topology map of the polyhedra and extended structures, in a Schläfli space, is illustrated and is discussed from the point of view of its organizational value for defining the topological relationship of structures from their Schläfli indices. A comment is then made with respect to the definition of the various vertex connectivities in structures, from knowledge of the circuit number of the vertex. It is shown here that vertices containing polar connections have a reduced circuit number from that calculated according to the prescription p(p-1)/2. Next a review is made of the Wells point symbols and corresponding Schläfli indices; first of the regular diamond and graphene nets; second of the semi-regular nets, including the Archimedean fullerene polyhedron and the Cooperite structure-type, and the Catalan fluorite and Waserite structure-types; and third of the irregular nets to include the Wellsean glitter and phenacite structure-types. The direct translation of the Wells point symbol to a weighted average polygonality, n, and a weighted average connectivity, p, is demonstrated in these examples.

* Corresponding author (castro@quimica.unlp.edu.ar / direccion@inifta.unlp.edu.ar)

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 [1] and its discovery marks the origin of the discipline of topology [2]. This relation is shown in Equation 1 below:

(1) $$V - E + F = 2$$

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 internal beauty, are idealized divisions of the sphere into the topology suggested first by Euler in his 1758 paper [1].

Some time after this, in a paper due to Schläfli, [3] the identities shown in Equation 2 and Equation 3 were discovered:

(2) $$nF = 2E$$

(3) $$pV = 2E$$

Schläfli identified the polygonality of convex polyhedra; or any division of the sphere into vertices, edges and faces; as the averaged number of sides of the polygonal faces in the considered object derived from the sphere. He determined the relation shown in 2, that the averaged polygonality in the 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 the Schläfli relation between the connectivity of convex polyhedra, p, 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 of the edges 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) there are differing numbers of edges to each polygonal face and/or differing numbers of edges meeting at each polygonal vertex in the polyhedron. One speaks of the semi-regular polyhedra, these are the Archimedean (polyhedra with more than 1 type of polygonal face) and Catalan (polyhedra with more than 1 type of polygonal vertex) polyhedra [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.

Schläfli substituted Equations 2 and 3 into the Euler relation (Equation 1), as shown in Equation 4, to obtain a relation between V, E and F; known as the primary topological indices; and n and p; known as the secondary topological indices.

(4) $$1/n - 1/2 + 1/p = 1/E$$

This latter Schläfli relation is important from the perspective of the Schläfli symbols (n, p) that can be identified for any polyhedral object. All polyhedra have rigorously determined values of n and p; just like they have rigorously determined values of V, E and F. The ordered pair thus formed of n and p, the polyhedral Schläfli symbol, represents a location in a Cartesian-like space, called a Schläfli space, in which the polyhedral object can be mapped.

Figure 1 shows the beginnings of this topological mapping for the regular polyhedra. The five regular polyhedra are called the Platonic solids for their role as elements in Plato's philosophical treatise known as the Timeas [5]. The polyhedron with the highest topology is the tetrahedron (meaning 4 equivalent faces) with the Schläfli symbol (3, 3). It marks the origin of this map [6]. Similarly, there is the cube (4, 3) and the pentagonal dodecahedron (5, 3); lining the column underneath the tetrahedron. To the right of (3, 3) are the octahedron (3, 4) and the icosahedron (3, 5). One can see immediately 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 polygonalities, n; the Catalan polyhedra have fractional connectivities, p; and the irregular polyhedra have both fractional polygonality and fractional connectivity.

In the 1950's Wells began his enumerative work on 2-dimensional (2D) and 3-dimensional (3D) networks and novel crystal structures [3]. He labeled his novel networks with the Schläfli symbols (n, p) to identify them. For while he did not determine a Schläfli-like relation for crystal structures; that is collections of vertices, edges and faces filling 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 unit of pattern of extended structures in both 2- and 3-dimensions [3]. He concluded that the topology map for the polyhedra, shown in Figure 1, could be extended in Schläfli-space by a simple augmentation of the ordered pairs of numbers (n, p), the Schläfli symbols, to the right of those for the polyhedra. Such an augmentation of this topology map involved moving into frontier that included the 2-dimensional networks, like the regular 2D extended structures of the graphene net (6, 3), the square net (4, 4) and the closest packed net (3, 6); and also the semi-regular and irregular tilings of the Euclidean plane, into the territory of the 3-dimensional networks. Figure 2 shows the extension of the topology map due to Wells. Note that to the right of the solid line, the 3-dimensional nets, the Schläfli symbol (n, p) may represent more than one way of filling space with a corresponding network of the specified topology.

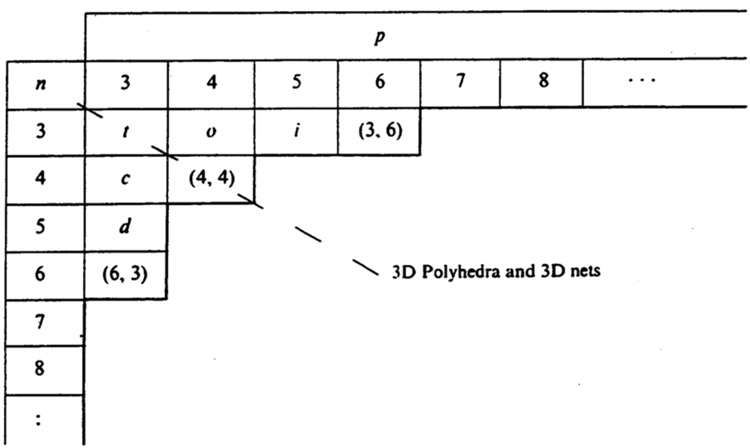

Figure 1: Partial topology map of the polyhedra and 2D regular structures.

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)	
⋮							

Figure 2: Complete topology map for the regular structures.

Early work by Wells involved the enumeration of the regular 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. Such networks, termed regular, represent structures with some of the highest possible topologies. This work included such topologies as that represented by the Schläfli symbol (7, 3) in which the polygonality of the circuits in the network, n, is uniform at 7, and the connectivity of the vertices in the network is uniform at 3 [7]. In this work, according to Wells, he was attempting to extend the topology map from (5, 3), the polyhedron called the pentagonal dodecahedron, to (6, 3) the 2D structure known as the graphene net, onto (7, 3) which represents a continuation of this sequence into 3-dimensional space. He eventually determined 4 distinct structures, 4 nets, that possessed the Schläfli symbol (7, 3) [6]. He did other similar elegant work on 3D networks of topology (8, 3), (9, 3), (10, 3) and (12, 3) [7].

Later on Wells turned to networks whose topology was lowered, these were the semi-regular and irregular 3D networks [4]. He introduced the Wells point symbols to represent the topology of these complex structures and it is the Wells point symbols that concern us in the present discussion. From the identification of the Wells point symbol for a network, one can in turn calculate the corresponding Schläfli symbol (n, p). This translation is important because the Schläfli symbol identifies the network and specifies its relative location with respect to all other networks in the topology map in Schläfli space. The Wells point symbol compactly summarises the polygonal circuitry that surrounds each of the p-connected vertices in the unit of pattern of a network (a model of crystalline material). The Wells point symbol also reflects the stoichiometry of the network. These ideas are described in the next Sections.

2. Comment on Circuit Numbers and Vertex Connectivity

There are two components to the mapping of structures in Schläfli space, as is shown in Figure 1 and 2 above. The polygonality is given the symbol n and it is derived from knowledge of the connectivities of the vertices, given by the symbol p, in the pattern of the structure. Of primacy in determining the Wells point symbol for a structure, and translating this point symbol into a Schläfli symbol (n, p), is the translation of the vertex connectivity in a structure from the circuit number about the vertex. The circuit number refers to the number of independent circuits that surround a particular point in the structural pattern. In a strict topological sense it would appear that circuit numbers for vertices would be given by Equation 5 [4]:

(5) $$\text{circuit \#} = p(p-1)/2$$

From this circuit number relation it would appear that a 3-connected point would have 3 circuits about it, a 4-connected point would have 6 circuits about it, a 5-connected point would have 10 circuits about it, and so on. This would strictly be the case if not for the polar circuits, those circuits formed by connections within the vertex 180° opposed from each other. One must correct the circuit number expression in Equation 5 for the number of these polar circuits in the vertex, called q. Equation 6 shows the correct expression for the circuit number about a given vertex:

(6) $$\text{circuit \#} = p(p-1)/2 - q$$

For example, consider a square planar vertex, as is shown in Figure 3 below. It would appear that such a vertex would have 6 independent circuits about it from inspection of all the pairs of connections that could possibly be drawn from the vertex.

In fact there are only 4 independent, non-polar pairs of connections that define the independent circuits about this vertex. The 2 polar pairs of connections do not play a role in the ultimate, actual topology of a structure containing this vertex. To see why this is so, consider an infinity proof as is outlined here for the square net.

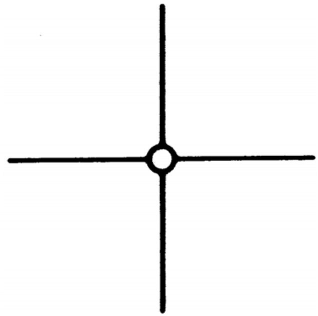

Figure 3: Square planar vertex topology.

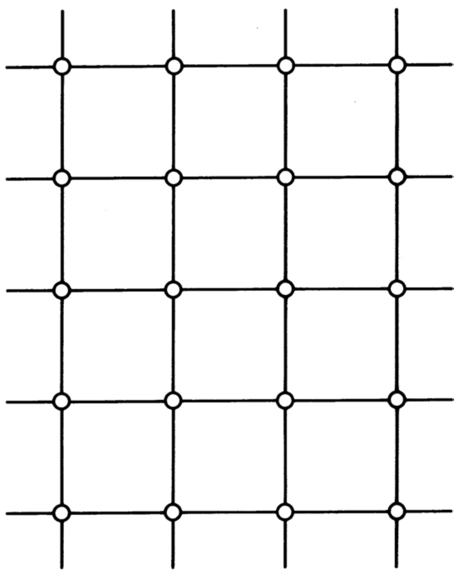

Figure 4: The square net (4, 4).

In the Wells point symbol the exponent is the circuit number, with a value of 4 it is understood to represent a structure composed of square planar vertices which are involved in four 4-gon circuits about each vertex in the structure of the square planar network. The base 4 is the polygonality of the circuitry. This all will be discussed more fully below.

From the Schläfli symbol (4, 4) it can be seen that the averaged polygonality, n, is 4 and the averaged connectivity, p, is 4, as well. This is easy to see in this case, because the network has a very regular topology. If one substitutes the values of $n = 4$ and $p = 4$ into the Schläfli relation shown in Equation 2 above, one sees that indeed the square net is a 2-dimensional extended structure which is infinite in extent. The infinite extent of the network is evident from Equation 2 because the number of edges, E, is calculated to be ∞.

Now, if one were to compute n and p by including the 2 polar pairs of connections, as is diagrammed in Figure 5.

One gets the same four 4-gons as in the previous analysis, and one, in addition, yields two 6-gons from forming the shortest circuits about the two polar pairs of connections. The corresponding Wells point symbol of the square net would appear to be $4^4 6^2$, where in this case we have a circuit number of 6 for the square planar vertex, this corresponds to the sum of the exponents in the Wells point symbol. In addition we have both 4-gons and 6-gons in the square net structural pattern.

We can translate the Wells point symbol into a corresponding Schläfli symbol of $(4^{2/3}, 4)$. The connectivity, p, of 4 arises from the fact that the square planar network is composed of 4-connected square planar vertices. The polygonality, n, is generated from taking a weighted average over the circuits present about each vertex in the net, such a calculation is shown in Equation 7:

(7) $$n = [4x4 + 6x2]/6 = 4^{2/3}$$

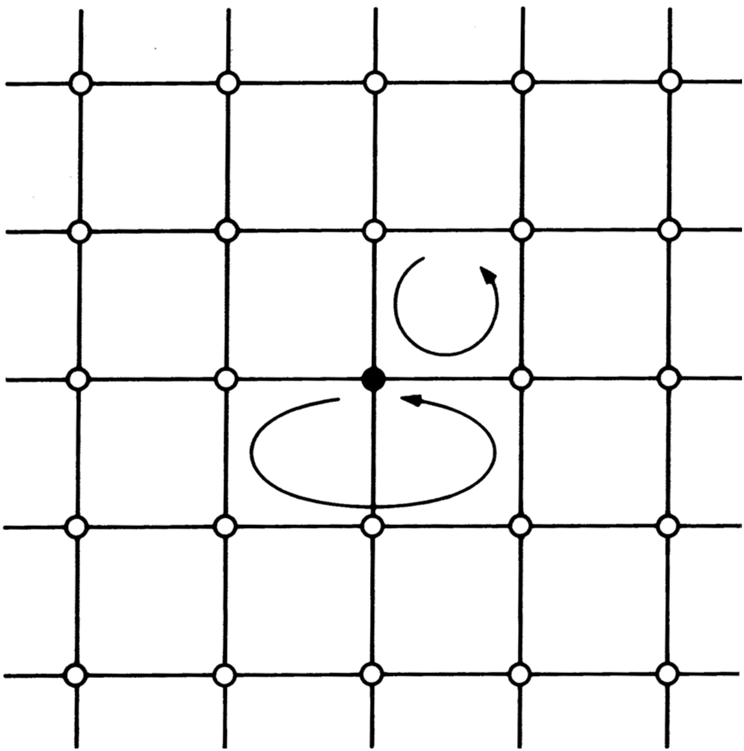

Figure 5: Alternative polygon analysis of the square net.

Now if we take the latter expression of the Schläfli indices and substitute into Equation 4, the Schläfli relation, one obtains the following equality for the infinite square planar network:

(8a) $$1/E = -0.03571$$

(8b) $$E = -28.00$$

Clearly, this result, the Schläfli symbol $(4^{2/3},4)$, is not consistent with the topology of the infinite square net as the number of edges is not ∞ but is in fact computed to be about –8. On the other hand, omitting the polar pairs of connections in the square planar vertex leads to a Schläfli symbol (4,4) which is consistent with the topology of the infinite square net as the corresponding number of edges is properly ∞. From inspection, then, we have tabulated the following rules for converting a circuit number into a vertex connectivity, in light of the infinitely proof, for the first 8 vertexes which are found to form common connectivity motifs in the structure of matter.

Connectivities of 7, 9, 10 and 11 are of course possible and will be explored elsewhere.

3. Wells Point Symbols for Regular Nets: Graphite and Diamond

We begin with the simple case of the topologically regular structures. Such structures are termed regular because all vertex connections are identical and all polygonal circuits are uniform as well. The graphite and diamond structure-types are the archetypal allotropic forms of carbon and are both topologically regular structures [8]. It is also true that graphite and diamond have both unusually high symmetries. The graphene sheet, shown in Figure 6, is the fundamental component of the graphite structure-type.

Table 1: Names, vertex connectivities and circuit numbers for the first 8 commonly occurring vertex topologies.

name	vertex connectivity	circuit number
trigonal planar	3	3
square planar	4	4
tetrahedral	4	6
trigonal bipyramidal	5	9
octahedral	6	12
body centered	8	24
10-connected	10	40
closest packed	12	60

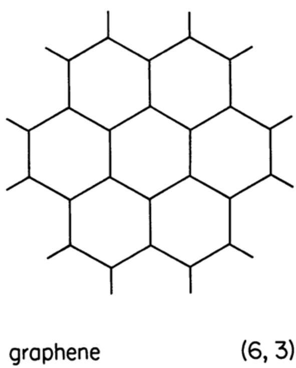

Figure 6: The graphene sheet (6, 3).

Such graphene sheets belong to the plane group p6mm [9]. They are layered onto each other in an alternating .....ABAB.... sequence to generate the rhombohedral graphite structure-type in space group R3c, number 167, and they are layered onto each other in an ....ABCABC.... sequence to generate the hexagonal graphite structure-type in space group $P6_3/mmc$, number 194 [10]. The topology of graphite is expressed fully through the component graphene sheets. Inspection of Figure 6 reveals that all the polygons in graphene are 6-gons and all vertices are 3-connected and trigonal planar. It is therefore a trivial matter to write down the Schläfli symbol for graphene, it is just (6, 3).

One can see its location in the topology map of Figure 2, it is just beyond (5, 3) the pentagonal dodecahedron, in the diagonal panel to the immediate left of the solid line that separates 3D structures from 2D structures. The graphene sheet is an archetypal tiling pattern used in honeycombs and in the interior decorating of homes and public buildings. The Wells point symbol corresponding to (6, 3) is 6^3. The similarity between the Schläfli symbol and the Wells point symbol for the graphene sheet is a bit deceptive, later examples will show that translation of the Wells point symbol into a Schläfli symbol for a network, which is the focus of this paper, is not usually so straightforward as this. From 6^3 we may first identify the connectivity, this point symbol is for a uninodal net, hence its simplicity, and we identify the exponent 3 in the point symbol as the circuit number belonging to the trigonal planar vertex. This translation was obtained from the data in Table 1 above.

To get at the polygonality, which we have already trivially identified as 6 from inspection of the sketch of the graphene sheet, one simply sums all the sides of all the polygonal circuits about the vertices in this uninodal net and divides by the number of polygonal circuits common to each such vertex. Such a computation is trivial in this case and is shown in complete form in Equation 9.

(9) $$n = 3x6/3 = 6$$

The unit cell of the cubic diamond lattice is shown in Figure 7, it lies in space group Fd3m, number 227. The lattice can be envisioned as a sequence of ......ABCABC......layering of carbon atoms, or alternatively as a stacking of all chair cyclohexaneoid units to fill 3D space.

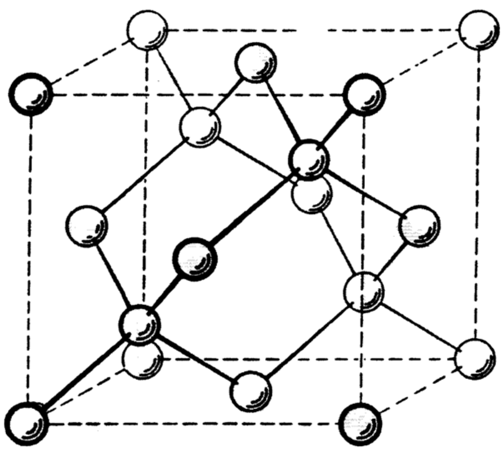

Figure 7: The cubic diamond lattice (6, 4).

Yet another polytype of diamond is known as hexagonal diamond, or Lonsdaleite after the famous British crystallographer. Hexagonal diamond lies in space group P63/mmc, number 194, like hexagonal graphite, and possesses a stacking sequence of carbon atoms in the pattern .....ABAB.....The topology of all diamond polytypes is the same, as will easily be revealed in an extended drawing or by building models [10].

Inspection of Figure 7 reveals all carbon atoms are tetrahedral, therefore the diamond net is uninodal and the circuit number of the tetrahedral vertex can be identified from Table 1 as 6. There are 6 circuits emanating from the tetrahedral vertices in diamond. By drawing extended sketches of the lattice, so that the 6 circuits of one of the tetrahedral nodes can be traced, it will become obvious that the polygonal circuits, all 6 of them, are 6-gons. The Wells point symbol for diamond is therefore 6^6. It is an easy matter to translate the point symbol into the Schläfli symbol (6, 4). The computation of n for diamond is shown in Equation 10.

(10) $$n = 6x6/6 = 6$$

4. Wells Point Symbols for Semi-Regular Nets

Archimedean Structures

The Archimedean polyhedra, and related 2D and 3D structures, are semi-regular structures in that they consist of uniform vertex connections while possessing more than one type of polygonal circuit in their structures. As such, the Archimedean structures will have integer vertex connectivity in the Wells point symbol and corresponding Schläfli symbol, and fractional polygonality. We begin with an evocative example of modern day topology at work, this the famous molecule known as Buckminsterfullerene [11]. Figure 8 shows a drawing of the carbon allotrope, it is in the icosahedral symmetry point group I_h. By inspection one can write down the Wells point symbol.

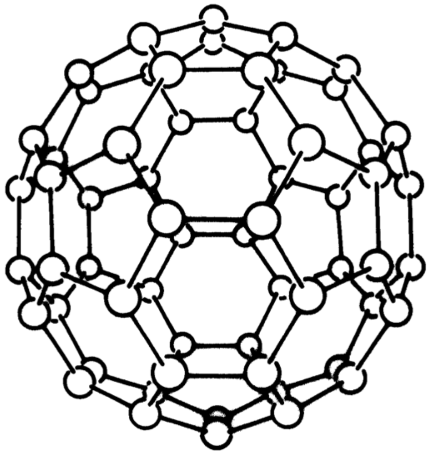

Figure 8: The Archimedean Buckminsterfullerene polyhedron ($5^{2/3}$, 3).

The net is uninodal with all vertices 3-connected, quasi-trigonal planar. From Table 1 it is clear that the exponent in the Wells point symbol for this structure will be 3. However, due to its Archimedean nature, there are indeed two types of polygons common to each 3-connected vertex. One can see that two 6-gons and one 5-gon meet at each vertex. It is a simple matter to represent this in a point symbol as (56^2). The exponent for the 5-gons is just 1 where we leave this out, the exponent for the 6-gons is 2. One can see immediately that the sum of the exponents, 2 + 1, is in fact equal to 3 as it must be for trigonal planar connectivity.

To get at the polygonality for the structure, one needs to take a weighted average over the circuitry about the uninodal, trigonal planar vertices. This is accomplished by summing the products of all the exponents multplied by their respective bases and dividing by the sum of the exponents, as is shown in gory detail in Equation 11.

(11) $$n = [(1x5) + (2x6)]/3 = 5^{2/3}$$

Therefore the Schläfli symbol for Buckminsterfullerene is just ($5^{2/3}$, 3) [12].

As an example of an extended structure which is Archimedean, one may consider the Cooperite structure-type which is the structure of PtS and PdO [13]. It is a tetragonal structure-type in the space group $P4_2/mmc$, number 131. The net is shown in Figure 9 where one notes immediately that the structure consists of a mixture of tetrahedral and square planar vertices. Technically, it would be considered an irregular net as the vertices are not equivalent, and it consists of more than one kind of polygonal circuit. However, as the tetrahedral and square planar vertices are both 4-connected, we can consider it to nominally be Archimedean

.

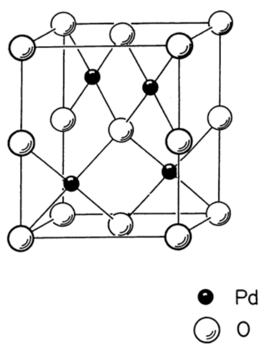

Figure 9: The Archimedean Cooperite network ($6^{2/5}$, 4).

To get at the Wells point symbol we first note its stoichiometry. As is evident in Figure 9 there is a 1 to 1 ratio of square planar to tetrahedral vertices in the net. A point symbol will need to be written down which consists of two brackets, one to indicate the topology about the square planar vertex, and one to indicate the topology about the tetrahedral vertex. Further, the sum of the exponents in the first bracket should be equal to 4, as this is the circuit number translation for square planar connectivity from Table 1. Similarly from Tabel 1, the bracket representing the tetrahedral vertex should have exponents that add to 6.

In order to visualize the circuitry about the two vertices in this binodal network, it is just necessary to resort to sketches that show completely the polygonal circuits about all 4 non-polar connection pairs in the square planar node, and all 6 connection pairs in the tetrahedral node. Upon analyzing sketches one sees that there are two 4-gons and two 8-gons about the square planar node, and there are two 4-gons and four 8-gons about the tetrahedral node. The Wells point symbol is just $(4^2 8^2)(4^2 8^4)$ for Cooperite. One can obtain the polygonality, n, in the manner just outlined in the case of the Archimedean Buckminsterfullerene polyhedron, above:

(12) $n = [(2x4) + (2x8) + (2x4) + (4x8)]/[2 + 2 + 2 + 4] = 6^{2/5}$

The connectivity index, p, is just 4 as Table 1 reveals. Therefore, the Schläfli symbol is given by $(6^{2/5}, 4)$.

Catalan Structures

The Catalan polyhedra were discovered in the 19th century after the Archimedean polyhedra had been enumerated in Ancient Greece more than 2000 years before. The Catalan polyhedra are known as the duals of the

Archimedean polyhedra. This is evident from the Schläfli symbol of the polyhedron where the following duality relationship holds [3][5]:

(13) $$(n, p) = (p, n)_{dual}$$

Being the duals of the Archimedean polyhedra, the Catalan polyhedra possess more than one type of vertex and uniform polygonal circuits in their structures. Thus, in the Schläfli index of a Catalan structure, the polygonality will be integer and the connectivity will be fractional.

The Catalan polyhedra can be constructed from their dual Archimedean polyhedron counterparts by joining the midpoints of all adjacent faces together. Such a reciprocal construction exists in 2D as well, where the square net (4, 4) is self-dual and the hexagonal net can be tesselated inside the close packed net and vice versa. This reciprocity extends to the semi-regular plane tilings as well. Although, formally, there exist dual relationships of the 3-dimensional networks; like (6, 4), the Schläfli symbol for the diamond net, is the 3D dual of (4, 6), the primitive cubic net; the construction of one 3D net from the other by joining midpoints of adjacent faces together is not, in practice, possible.

Here is described the translation of the Wells point symbol to the corresponding Schläfli symbol for two Catalan extended structures. Perhaps it would have been illustrative to show a translation of a Catalan polyhedron, but the extended structures are more complex and illustrate the process of translation more fully. Shown in Figure 10 is the fluorite structure-type, this is a Catalan network. It is a cubic structure-type in space group Fm3m, number 225 [14].

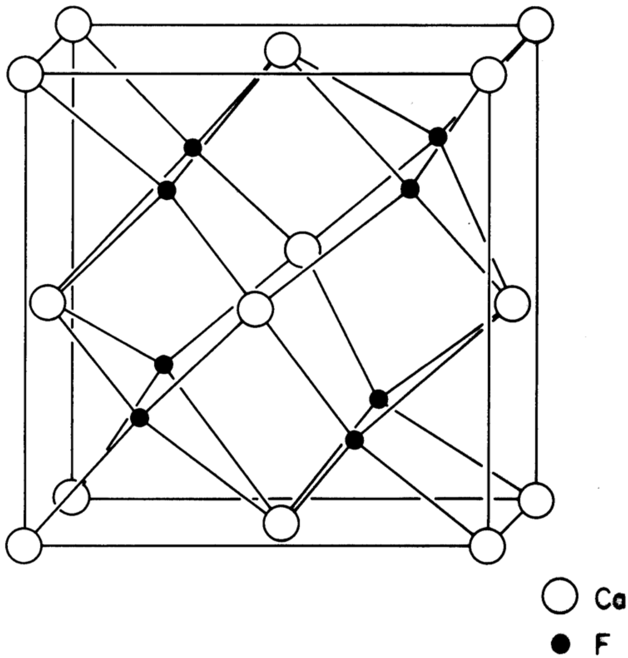

Figure 10: The Catalan fluorite lattice (4, $5^{1/3}$).

One can see by inspection in the drawing that there are eight tetrahedral 4-connected points in the unit cell and four body centered 8-connected points in the unit cell. The stoichiometry is thus AB_2, with A being 8-connected and B being 4-connected.

By drawing a sketch of an extension of the fluorite unit cell showing the complete circuitry about one of the body centered lattice points and one of the tetrahedral lattice points, one can identify the polygons within the Wells point symbol for this complex network. Inspection of such a sketch reveals the simplicity of the topology of fluorite as all polygonal circuits in the structure-type are 4-gons. At first sight this sketching seems a bit involved as there are 24 independent connection pairs about the 8-connected body centered vertices in the lattice, but in fact the tracing is straightforward. The Wells point symbol is immediately written down as $(4^{24})(4^{6})_2$. The exponents in the point symbol reveal the vertex connectivities of the vertices in fluorite. From Table 1 we see that a circuit number of 24 corresponds to an 8-connected body centered vertex, and 6 is the circuit number for the 4-connected tetrahedral vertex. Note the additional coding of the 1 to 2 stoichiometry of body centered to tetrahedral vertexes by the inclusion of the proper subscripts in the point symbol. Finally, the bases in the point symbol, which refer to the relative occurrences of the polygonal circuits, are all 4. This is in keeping with the fluorite structure-type being a Catalan network.

To get at the polygonality, n, one simply sums the products of the stoichiometric subscript factors with the corresponding circuit numbers and the corresponding polygonalities and divides by the number of polygons so coded, this is given by the sum of the products of the stoichiometric subscript factors with the corresponding circuit numbers:

(14) $$n = [(1x24x4) + (2x6x4)]/[(1x24) + (2x6)] = 4$$

The connectivity, p, is gotten by taking a weighted average of the relative connectivities in the unit cell considering the stoichiometric subscript factors and the translation of the circuit numbers in the exponents of the point symbol into vertex connectivities. The denominator in such an expression is the sum of the vertexes in the stoichiometric formula unit:

(15) $$p = [(1x8) + (2x4)]/3 = 5^{1/3}$$

Hence, the Wells point symbol $(4^{24})(4^{6})_2$ is translated into the Schläfli symbol $(4, 5^{1/3})$.

The unit cell of the Catalan network of Waserite, Pt_3O_4, is shown in Figure 11 below. It is a 3-,4-connected cubic structural pattern in space group Pm3n, number 223 [15].

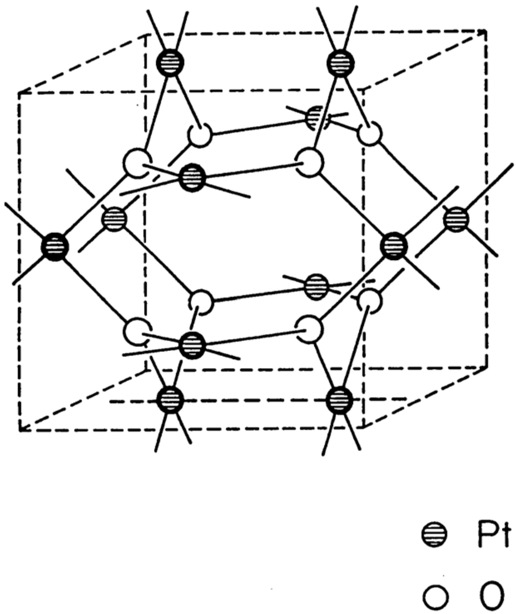

Figure 11: The Catalan Waserite network (8, 3.4285).

One can see immediately on inspection of the unit cell that there are six 4-connected square planar vertices and eight 3-connected trigonal planar vertices in the unit cell. It is a beautiful example of a 3-,4-connected network because of its high cubic symmetry and that it displays strain-free ideal bond angles of 90° and 120° about the square planar and trigonal planar vertices, respectively.

By drawing an extended sketch of the Waserite unit cell, one can trace the 3 polygonal circuits about the trigonal planar vertices and the 4 polygonal circuits about the square planar vertices, respectively. The relative simplicity of the topology of Waserite is revealed in such an analysis as all shortest polygonal circuits about all vertices are 8-gons. It is an octagonal structure-type. From the stoichiometry identified above, one can immediately write down the Wells point symbol for the network as $(8^4)_3(8^3)_4$, where the exponents and subscripts are seen to correspond the six 4-connected square planar vertices in the unit cell to eight 3-connected trigonal planar vertices in the Waserite unit cell. The matter of translation is trivial, the value of n and p are indicated in Equations 16 and 17:

(16) $$n = [3x4x8) + (4x3x8)]/[(3x4) + (4x3)] = 8$$

(17) $$p = [(3x4) + (4x3)] / 7 = 3.4285.......$$

Hence, the Schläfli symbol for Waserite is simply (8, 3.4285). Here the connectivity shows up as a continued fraction.

5. Wells Point Symbols for Irregular Nets

Finally, we turn to the topologically irregular structures. These structures have been previously labeled as the Wellsean structures [8]. The structures are labeled irregular, or Wellsean, because they consist of more than one type of vertex connectivity and they possess more than one kind of shortest polygonal circuit about one or the other, or both, vertices. Such structures, therefore, contain fractional polygonality and fractional connectivity in their structural pattern. It is important to point out at the beginning that there may, in fact, be more complex networks than this, including those with more than 2 distinct vertex connectivities.

As the first example of such a network, we consider the glitter structure-type first published in 1994 [16]. An extended view of the glitter structure is shown in Figure 12 below:

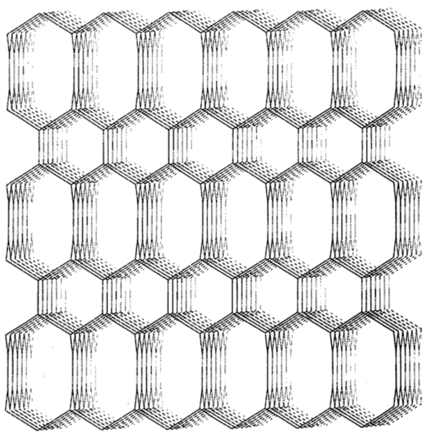

Figure 12: Extended view of the topologically irregular glitter network with the corresponding Schläfli symbol of $(7, 3^{1/3})$.

The structure is of tetragonal symmetry, in space group $P4_2/mmc$, number 131. It is interesting in this connection that the space group of Cooperite is identical to that of glitter. In fact one can move from the Cooperite structure-type to the glitter structure-type by replacing the 4-connected square planar vertices with 3-connected trigonal planar atom pairs. It is an elementary topological substitution of the type of which Wells was a master designer.

Figure 13 shows the elementary unit cell of glitter. One can see by inspection of the unit cell that there are four 3-connected trigonal planar vertices for every two 4-connected tetrahedral vertices.

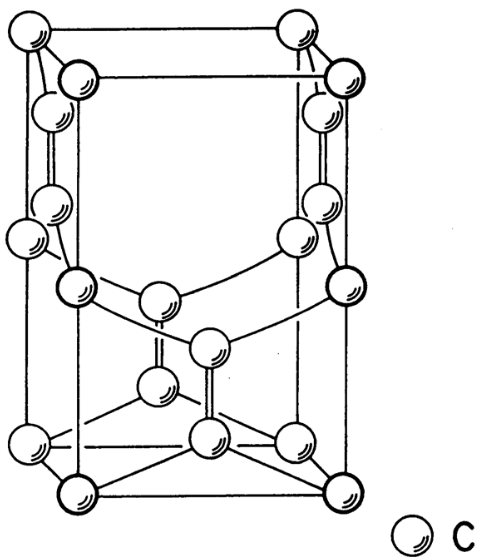

Figure 13: Unit of pattern of the topologically irregular glitter network with the Schläfli symbol of $(7, 3^{1/3})$.

The stoichiometry of the lattice is therefore 1 to 2 tetrahedral vertices for trigonal planar vertices. From Table 1 we know that there are indeed 6 polygonal circuits about the 1 tetrahedral vertex in the stoichiometry, and 3 polygonal circuits about each of the 2 trigonal planar vertexes in the stoichiometry of glitter. The point symbol about the trigonal planar vertices is trivial to work out from an extended sketch of glitter, as two 6-gons and one 8-gon meet at each such vertex in the pattern. The partial point symbol about the trigonal planar vertices is thus $(6^2 8)$. Working out the tetrahedral point symbol requires more work, because there are 6 polygonal circuits about these vertices. By sketching and carefully tracing, one can see that the partial point symbol for the tetrahedral connections in glitter is $(6^2 8^4)$.

By specifying the stoichiometry of glitter, the Wells point symbol is established from these two parts as $(6^2 8^4)(6^2 8)_2$. One can immediately get at the averaged polygonality and connectivity in the unit cell of glitter, as is shown in Equations 18 and 19:

(18) $n = [(1x2x6)+(1x4x8)+(2x2x6)+(2x1x8)]/[(1x2)+(1x4)+(2x2)+(2x1)]= 7$

(19) $p = [(1x4) + (2x3)] / 3 = 3^{1/3}$

Hence one can see that the Schläfli symbol is just $(7, 3^{1/3})$ for glitter [17]. It appears to correspond to the Schläfli symbols for the Catalan networks because its polygonality is integer. However, as the Wells point symbol reveals, it is an irregular net consisting of 3- and 4-connected points in 6- and 8-gon circuits.

The phenacite structure-type was discovered in 1930 by Bragg et al. [18]. It is a challenging structure-type consisting of trigonal planar 3-connected vertices and tetrahedral 4-connected vertices that alternate in 3-dimensions to form a hexagonal structural pattern. The unit cell is shown in Figure 14, the structure belongs to space group $P6_3/m$, number 176.

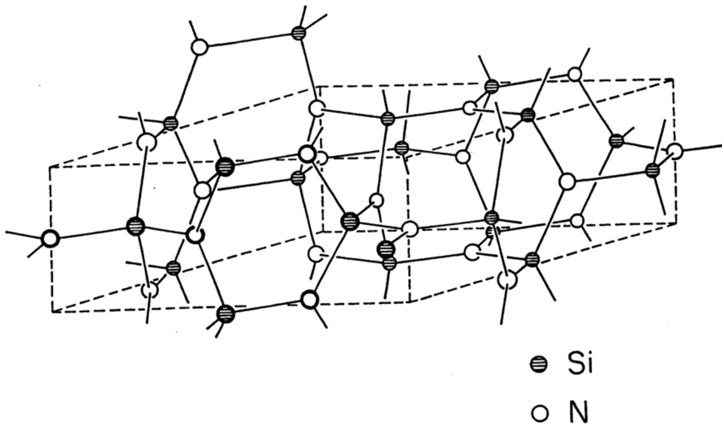

Figure 14: Unit of pattern of the topologically irregular phenacite network with the Schläfli symbol ($6^{4/5}$, 3.4285).

It clearly requires concentration to see that the stoichiometry of this topologically irregular network is four trigonal planar 3-connected vertices to three tetrahedral 4-connected vertices. Also it would be difficult to draw an accurate extended sketch of such a complex structure to get at the polygonal circuits in the structure, but one can build an extended model and from this identify those polygonal circuits. There are thus, topologically, 3 types of vertex in the phenacite structure type. Two types of circuitry about

3-connected trigonal planar atoms and one type of circuitry about the 4-connected tetrahedral atoms. One can see this in Figure 13 if one concentrates.

The Wells point symbol for the phenacite structure-type is given by $(6^3)_6(8^3)_2(6^38^3)_6$. [4] Therefore we have a 3 to 1 ratio of trigonal planar vertices with all 6-gon and all 8-gon circuitry about them, respectively. And we have three 4-connected tetrahedral formula units with the topology (6^38^3) in its circuitry. Note, as in Table 1, the exponents in the tetrahedral vertex point symbol add to a circuit number of 6, as they must. It is an easy matter now to translate this complex point symbol into a Schläfli symbol for the network as is shown in Equation 20 and 21:

(20) $n = [(6x3x6)+(2x3x8)+(6x3x6)+(6x3x8)]/[(6x3)+(2x3)+(6x3)^2] = 6^{4/5}$

(21) $p = [(6x3) + (2x3) + (6x4)] / 14 = 3.4285........$

Hence the Schläfli symbol for phenacite is $(6^{4/5}, 3.4285)$. It is indeed a Wellsean network with a fractional polygonality and a fractional connectivity. It is interesting here to see that the connectivity of phenacite is the same continued fraction, 3.4285........, as in the much simpler Waserite structure-type. This is because the stoichiometries of these two 3-,4-connected nets are identical at A_3B_4, where A is 4-connected and B is 3-connected.

REFERENCES

1. *Elementa doctrinae solidorum et Demonstratio nonnularum insignium proprietatum quibus solida heddris planis inclusa sunt praedita*, L. Euler, included in the Proceedings of the St. Petersburg Academy, 1758.

2. M. Henle, A Combinatorial Introduction to Topology, 1st Edition, W.H. Freeman and Company, San Francisco, CA, 1979, p.9.

3. A.F. Wells, The Geometrical Basis of Crystal Chemistry: (a) Part 1, A.F. Wells (1954) *Acta Crystallogr.*, **7**, 535. (b) Part 2, A.F. Wells (1954) *Acta Crystallogr.*, **7**, 545. (c) Part 3, A.F. Wells (1954) *Acta Crystallogr.*, **7**, 842. (d) Part 4, A.F. Wells (1954) *Acta Crystallogr.*, **7**, 849. (e) Part 5, A.F. Wells (1955) *Acta Crystallogr.*, **8**, 32. (f) Part 6, A.F. Wells (1956) *Acta Crystallogr.*, **9**, 23. (g) Part 7, Wells, A.F. and Sharpe, R.R. (1963) *Acta Crystallogr.*, **16**, 857. (h) Part 8, A.F. Wells (1965) *Acta Crystallogr.*, **18**, 894. (i) Part 9, A.F. Wells (1968) *Acta Crystallogr.*, Section B, 50. (j) Part 10, A.F. Wells (1969) *Acta Crystallogr.*, Section B, 1711. (k) Part 11, A.F. Wells (1972) *Acta Crystallogr.*, Section B, 711. (l) Part 12, A.F. Wells (1976) *Acta Crystallogr.*, Section B, 2619. (m) A.F. Wells, Three Dimensional Nets and Polyhedra, 1st Edition, John Wiley and Sons Inc., New York, 1977. (n) A.F. Wells, Further Studies of Three-dimensional Nets, American Crystallographic Association, Monograph Number 8, 1st Edition, American Crystallographic Association Press, 1979. Note that unfortunately the author could not locate direct references to the work of Schläfli in topology, the references to Wells are indirect but refer to Schläfli's work.

4. A.F. Wells, Further Studies of Three-dimensional Nets, American Crystallographic Association, Monograph Number 8, 1st Edition, American Crystallographic Association Press, 1979.

5. (a) M. Wenninger, Dual Models, 1st edition, Cambridge University Press, 1983. (b) P.J. Frederico, "Descartes on Polyhedra: A Study of the De Solidorum Elementis", appearing in Sources in the History of Mathematics and Physical Sciences 4, 1st edition, Springer-Verlag, 1982.

6. A.F. Wells, Three Dimensional Nets and Polyhedra, 1st Edition, John Wiley and Sons Inc., New York, 1977.

7. A.F. Wells, *Acta Crystallogr.*, **7**, 535 (1954).

8. M.J. Bucknum, *Carbon*, **35(1)**, 1, (1997).

9. C. Hammond, Royal Microscopical Society Microscopy Handbooks (19): Introduction to Crystallography, Revised Edition, Oxford University Press, Oxford, U.K., 1992, p.29.

10. (a) K.E. Spear, A.W. Phelps, and W.B. White, *J. Mat. Res.*, **5(11)**, 2277, (1990). (b) K.E. Spear, *J. Am. Cer. Soc.*, **72(2)**, 180, (1989).

11. J. Baggott, Perfect Symmetry: The Accidental Discovery of Buckminsterfullerene, 1st edition, Oxford University Press, Oxford, U.K., 1996.

12. This Schläfli symbol for Buckminsterfullerene, ($5^{2/3}$, 3), represents a correction to that erroneous symbol published as ($5^{5/8}$, 3) previously, see reference 8.

13. F.A. Bannister, *Z. Krist.*, **96**, 201, (1937).

14. R. W. G. Wyckoff, Crystal Structures, 2nd edition, Robert E. Kreiger Publishing Company, Malabar, FL, 1986, Volume I, p.239.

15. (a) E.E. Galloni and A.E. Roffo, *J. Chem. Phys.*, **9**, 875, (1941). (b) J. Waser and E.D. McClanahan, *J. Chem. Phys.*, **19**, 413, (1951).

16. M.J. Bucknum and R. Hoffmann, *J. Am. Chem. Soc.*, **116**, 11456, (1994).

17. This Schläfli symbol for glitter, (7, $3^{1/3}$), represents a correction to that erroneous symbol published as ($6^{2/3}$, $3^{1/3}$) previously, see reference 8.

18. W.L. Bragg and W.H. Zachariasen, *Z. Krist.*, **72**, 518, (1930).