Lederberg (II)

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Interim Report to the
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DENDRAL-64

A SYSTEM FOR COMPUTER CONSTRUCTION, ENUMERATION AND NOTATION OF ORGANIC MOLECULES AS TREE STRUCTURES AND CYCLIC GRAPHS

Part II. Topology of Cyclic Graphs

Introduction

Part I showed the canonical formulation of those chemical graphs which are pure trees. In Part II we introduce the formulation of pure rings, i.e. strictly cyclic graphs, each defined as a set of atoms not separable by less than two cuts. Part III will relate this topological analysis to the representation of complete structures. These are trees on which each ring will be regarded as a special node.

submitted by

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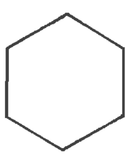
PART II. December 15, 1965

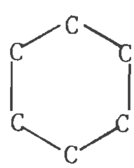
PART II. TABLE OF CONTENTS

This part consists mainly of an analysis of cyclic graphs to allow the enumeration of the ring structures of chemistry. Many chemical graphs are mixed, that is are trees in which cyclic subgraphs are embedded. The complete representation of such structures is taken up in Part III, and we will be concerned here only with the fundamentals of pure cyclic graphs. 2.00

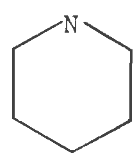
The most frequent ring in organic chemistry is the simple cycle, e.g., benzene; and these structures (ring structures with one ring) afford no special problems as they are simple mappings of a linear chain. A canonical form would be the cut which maximizes the DENDRAL value of the string. The encoding of the following figures is self evident: 2.01



i.e.,



(-6)



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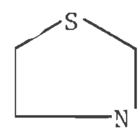
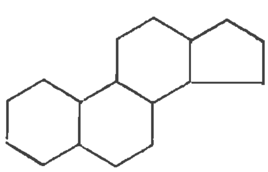


(-S.C.N.2)

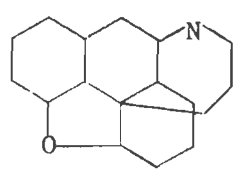
2.02

Polycyclic structures such as



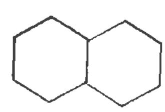
STEROID NUCLEUS

[4]



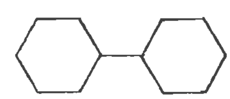
MORPHINE NUCLEUS

[5]



NAPHTHALENE

[2]



BIPHENYL

[1], [1]

are, however, quite important and require a more elaborate treatment. The chemist refers to a ring-structure (or "ring", when the context makes this clear) for a set of atoms inseparable by a single cut. The number of rings (bracketed above) in such a structure is the minimum number of cuts needed to convert the structure to a tree. For a polyhedron (a planar graph everywhere at least 3-connected), this is one less than the number of faces, i.e., the number of cuts needed to separate the graph, a definition we can generalize to 2-connected graphs as well.

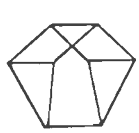
General Introduction to the Treatment of Rings.

Attempts to process rings on a node-by-node basis like linear DENDRAL 2.10
proved unrewarding. Ambiguities due to symmetry are usual, and many paths can be evaluated only by recursively searching through the entire graph. This approach was therefore abandoned in favor of a fundamental classification of the possible graphs. That is, the distinct ways in which a set of nodes can be connected to form a cyclic graph have been calculated in advance. To apply these calculations to actual formulas, a number of simplifying steps are introduced:

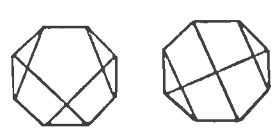
1. Analyze the ring into its paths and vertices (branch points). The 2.11
classification then depends on the set of branch points, the atoms which are triply connected. Organic rings rarely have more than three branches at any point; instances of four branches (usually called "spiro" forms) can be accommodated by exception. H atoms and other substituents attached to the ring are ignored.

2. Produce a general classification of connectivity diagrams, the trivalent 2.120
graphs. Section 2.2 reviews how the set of trivalent graphs can be systematically arranged without isomorphic redundancies. With few exceptions, such graphs are most conveniently presented as chorded polygons. (Hamilton circuits).

Polygonal graphs are relatively easy to compute, but they fail to show many
of the symmetries of the figures. This is dramatized by the two isomorphic 2.121
polygonal representations of the bi-pentagon.

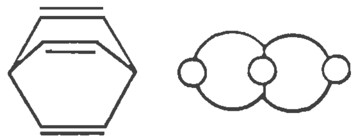


BI-PENTAGON



Furthermore, a few graphs lack Hamilton circuits, and thus cannot be represented 2.122

as chorded polygons.

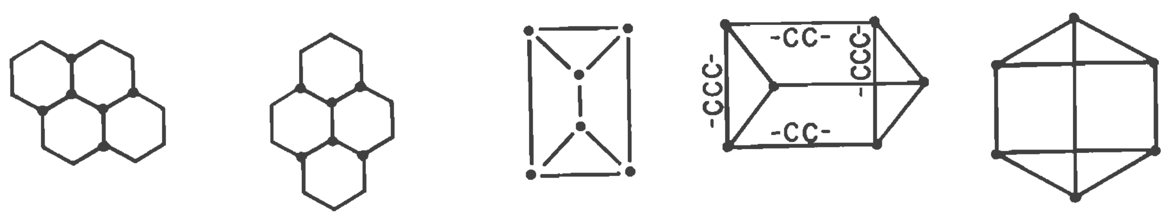


2.13

3. Map the paths of the chemical graphs on the diagram, according to the canons detailed below.

An example will be introduced at this point to help illuminate these detailed rules. 2.140

To recapitulate, the linear paths and the vertices connecting them are first identified. The vertices are simply the branch points, i.e., the atoms with three or more links to the rest of the ensemble. For these purposes a double or triple bond is a single link. The paths are then the intervals between the vertices. A path may be a simple link or a linear string of tandemly linked atoms. For example, marking the paths of pyrene (a) gives the diagram (b) 2.141 2.142



PYRENE

(a) (b) (c) (d)

which is readily recognized as isomorphic to the prism (c) and its formal graph (d). The isomorphism of (b) with (c) could also be established algorithmically by systematic permutation of the incidence matrix of the graphs. 2.143

(c) represents the essential idea of topological mapping. It then remains to describe a syntax for describing such a figure in a unique code in computable format. Part II concerns itself only with the possible vertex groups, leaving the mapping of the paths to Part III.

THE TRIVALENT CYCLIC GRAPHS 2.2

(The non-separable connections of n trivalent objects)

Each link must terminate in 2 nodes; each node has 3 incident links. 2.21
Hence there will be 3n/2 links and the order n must be even. The following development treats n from 0 to 12 in detail, but could be generalized indefinitely. The main objectives are to indicate

(1) all the possible graphs

(2) isomorphisms of superficially different graphs

(3) symmetries within a graph

(4) rational description of each item

(5) rational ordering of the graphs

(6) rational numbering of the vertices and paths

(7) compact, computable notation for each feature

2.22

Several computer programs have been applied together with substantial manual effort to meet these objectives. The results are mainly summarized in the accompanying diagrams.

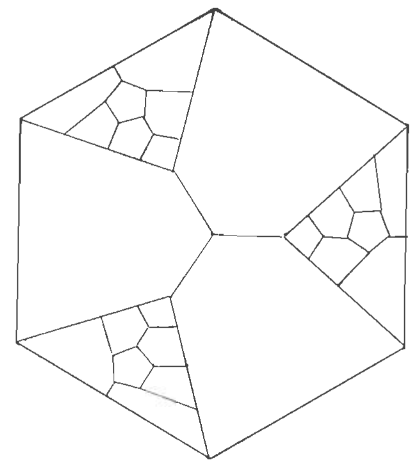
Any trivalent graph of a given order is found to represent either

(1) a polyhedron of the same order (i.e. a planar graph nowhere separable by < 3 cuts), or

(2) a compound graph, the union of two planar graphs of lower order, obtained by cross-reuniting a pair of cut edges, one from each graph, and thus somewhere separable by 2 cuts, or

(3) a gauche or nonplanar graph, also called skew.

Polyhedra, including the degenerate forms with 0 vertices (the circle with two virtual faces, no solid angles) and 2 vertices ("bicyclane", three virtual faces), are thus fundamental to the general development. For their formal computation we have relied on the conjecture that every trivalent polyhedron has a Hamilton circuit, i.e., a circuit of paths that traverses each vertex just once. On this basis, any polyhedron can be projected as an n-gon, with n/2 chords planted across all the vertices. (Therefore, graphs with a Hamilton circuit may be called "polygonal".) This conjecture has been attributed to Tait[1] by Tutte[2], who has found a counter example which has, however, 46 vertices[2]. While no tangible examples are known to have been missed, a sounder topological theory of polyhedra could be both reassuring and more elegant (see 2.5). 2.23



The trivalent polyhedra of from 0 to 12 vertices have been calculated in this way, and various representations of each of these are shown (Fig. 2T.5). They have also been checked for $n \leq 12$ by the traditional method of adding an extra edge in all possible ways to each of the faces of the polyhedra of order n-2. 2.231

The polyhedra were extracted as a subset of the chorded polygons. That is, all permutations of n/2 chords across an n-gon were systematically considered. This representation has the advantage that its elements remain invariant under manipulations of the polygon, e.g., rotation of the vertices. The program then demoted the graphs that had doubly connected parts, that is, that were <u>unions</u> of two graphs of lower order. All graphs were tested for isomorphisms by systematic tracing of the alternate paths to find other possibly distinct Hamilton circuits*, i.e., alternative representations as chorded polygons. Comparisons are made on the basis of span lists, i.e., cyclic lists showing the 2.232

*This is best accomplished by 2.90

span of the chord from each vertex (cf. 2.30).

The canonical form of the span list is the lowest numerical value* under the permitted operations of n-fold rotation and reflection. For the most part, the symmetries could be prospectively anticipated to make the program more efficient. The graphs were scrutinized for planarity (Kuratowski's criterion, see 2.25). The planar graphs were then candidates for manual construction of polyhedra. We conjecture that topological symmetry can always be carried over into the geometrical symmetry of the construction of the polyhedron. The assignment of solid angles is, of course, arbitrary.

* * * * *

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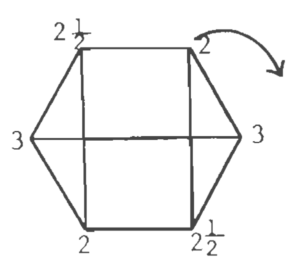
*2.2331

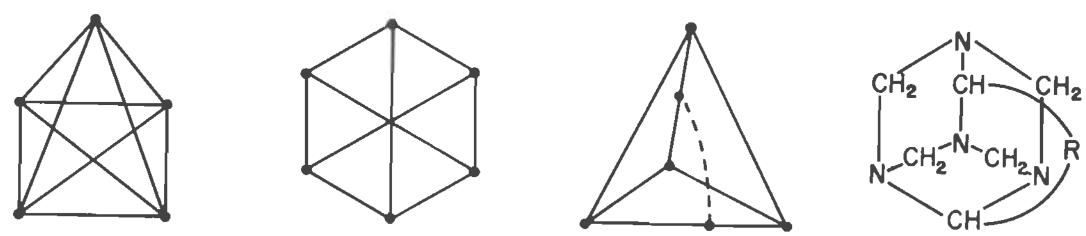
In the computations here, the program as it evolved included a particular interpretation of the span. This is the shortest interval between the nodes in either sense; when ambiguities were discovered, they were resolved by adding a low order bit (say 1/2) to the value for the retrograde sense. Hence for the prism the span values are:



Compound Graphs. Unions of smaller graphs have been developed in two ways. The program for permuting chord lists on the polygon produces all the compound graphs with Hamilton circuits. However, many compound graphs are non-polygonal. The only cases relevant to chemical graphs (i.e. with less than 38 vertices!) can be composed by a bilineal union of two circuits, when a single circuit is lacking. The theory of non-Hamiltonian polyhedra has some mathematical, if no chemical interest, and must be included in any general classification of graphs, as discussed in an appendix (2.72). 2.24

Gauche Graphs. A gauche or non-planar graph is one which cannot be represented on the plane (nor, therefore, by projection as a polyhedron), without some edge crossing over another. Kuratowski showed that any gauche graph must contain either (a) or (b): 2.250

Do such graphs play any role in chemistry? 2.251



(a) (b) (c) (d)

In fact, none of the 11,524 rings in the Ring Index is gauche; consequently, except for 6CCC, the gauche graphs have been deleted from the figures in this report. The consideration of 6CCC as a polyhedral derivative will illustrate the difficulties and possibilities of formulating a gauche structure. Fig. 2.25a can be passed over as a pentaspiro formation already of unreasonable, though perhaps not unattainable, complexity. 2.252

Figure 2.25c shows 6CCC as an internally chorded tetrahedron. That is, a gauche graph must have an additional path within an already tightly caged 2.253

structure. Figure 2.25d illustrates a possible candidate to fill this hiatus in topological chemistry.

The obligatory nonplanarity of the gauche graphs should not be confused 2.254 with the optional drawing of crossed paths in representations set out as alternatives to a planar mesh (v. Part III); a gauche graph has no planar mesh.

Interpretive Coding of Vertex Group Diagrams. 2.255

The chord list of any polygon can be abbreviated to give an interpretive code: (1) letters of the alphabet, A to Z, stand for spans from 1 to 26, (2) a chord is mentioned only once, when either end is first encountered, since the span fixes the location of the other end. Thus the prism, whose chord list is 234234 becomes 6BCB, the underscored figures referring to chords denoted by previous digits. Actually the last character is redundant, being fixed by its predecessors in the construction. Thus any polyhedron with n vertices, if it has a Hamilton circuit, can be constructively and compactly denoted with a code of only (n/2-1) characters. These codes, lacking invariance under rotation, are treacherous for the recognition of canonical forms and therefore play no role in the computation, being translated at once into the complete span list. These codes have also been shown on Figure 2T.5 for illustration purposes. The syntax will be evident from the examples and from the dissection of Figure 2T.20.

Ordering. The graphs are ordered by the following rather arbitrary 2.260 principles. There are however designed to facilitate matching of codes with established lists.

1. Polygons. The polygon is oriented so as to minimize the numbering 2.261 of its span list (cf. 2.2331). Within each series, the order is then given by the compact code generated from this number, v.s., 2.255. If two or more

polygons are isomorphisms, all are shown; the canonical choice among them has minimal coding.

A. **Polyhedra** are displayed first.

B. Then unions with polygonal representations.

2. Non-polygons. The polygons are projections of Hamilton circuits on a circle. When no single circuit captures all the nodes, the graph may be dissected into two disjoint circuits joined in a bilineal union (for further mathematical curiosities see 2.72). The canonical dissection creates a maximum couple of circuits, the larger taken first. The value of a circuit is determined by its

order (number of nodes)

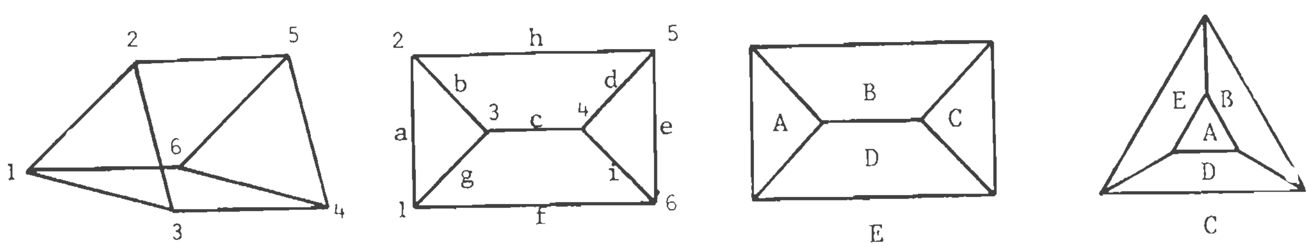
compact code: chord list (2.255)

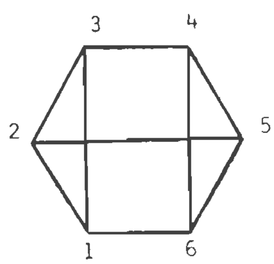
edge designated for splicing in bilineal union.

The coding follows the form $C_1:n_1,n_2:C_2$ where C_1 and C_2 are the component circuits; n_1 and n_2 are the spliced edges. The set of known examples for n=8, 10, 12, as given in 2T. 4 , will clarify the notation.

Numbering of Vertices and Edges. Before defining the mapping of paths we must consider the numbering, i.e. ordering the sequence of vertices and paths. This issue is closely connected with canonical orientation of the diagram. A natural linear order for the parts of a polyhedron is not always self-evident. The polygonal representation, whenever one exists, suggests one approach. We must still select an orientation of the polygon, which may offer a choice among n-fold rotational and 2-fold reflectional permutations. For the present treatment we adopt the minimum span list (See 2.2331). Thus, some possible representations and notations for the prism are: 2.30

2.31





SPAN LIST - 234234

CHORDLIST - 6BCB

INCIDENCE MATRIX

	2	3	4	5	6
1	1	1			1
2		1		1	
3			1		
4				1	1
5					1

FACE INCIDENCE (DUAL GRAPH) - BDE ACDE BDE ABCE ABCD

	B	C	D	E
A	1		1	1
B		1	1	1
C			1	1
D				1

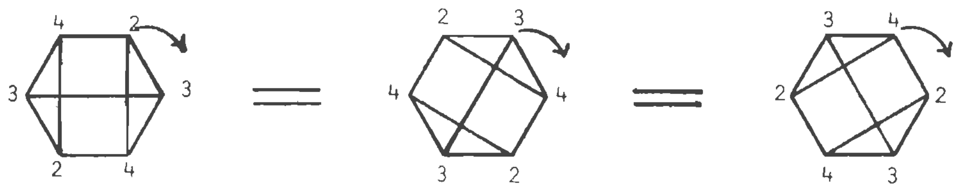
FACE LIST, VERTICES - 123 2345 456 1346 1256

FACE LIST, EDGES - abg bcdh dei efgi aefh

INTERCHANGE GRAPH - bfgh acgh bdgi cchi dfhi abgi abef abde cdef

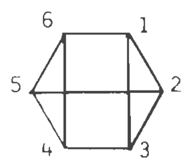
	b	c	d	e	f	g	h	i
a	1				1	1	1	
b		1				1	1	
c			1			1		1
d				1			1	1
e					1		1	1
f						1		1

Of these various representations, the span list is brief and, being invariant under rotation, easy to permute. We therefore denote each graph by its span list in minimal form and label the vertices in the corresponding sequence. Thus (234234) = (342342), of which (234234) is minimal. Hence 2.32



The numbers above are the span, not tne vertex values.

2.33

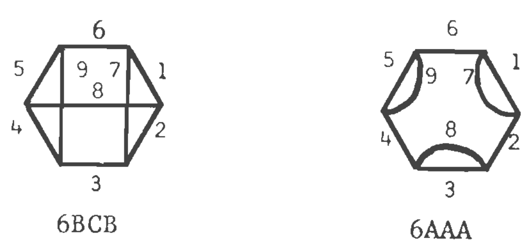


Vertex Labels

2.34

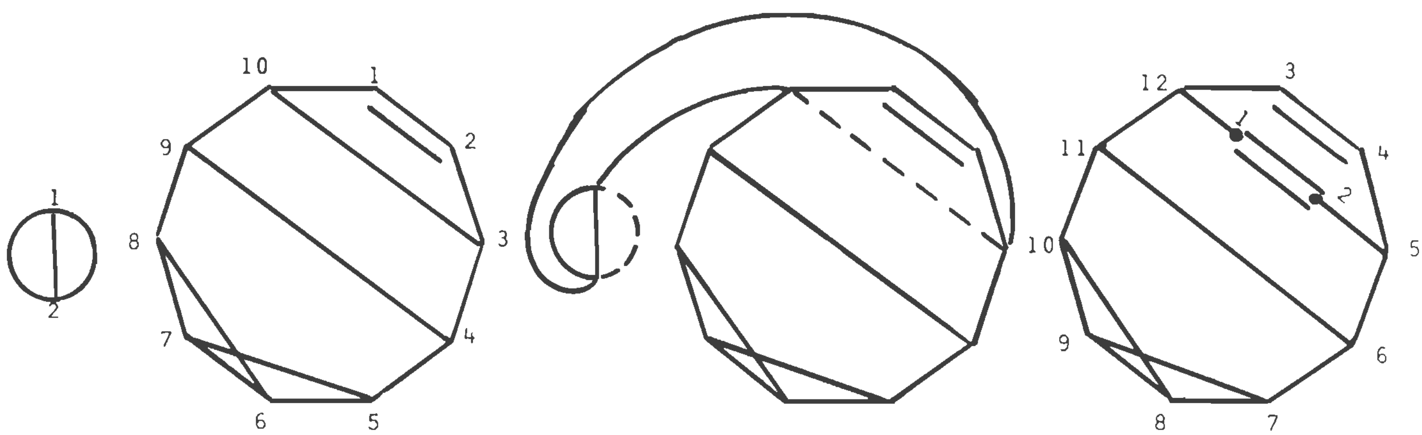
The vertices being numbered, the path list is in the order of the vertex couples, the polygonal circuit being taken first, then the chords. Thus the nine edges of the prism are, in order, 12, 23, 34, 45, 56, 61, then 13, 25 and 46. Caution: the polarity of each path follows this numbering. The same rule is applied to "self-looped edges," or "slings", i.e. chords with a span of 1. Examples:

2.35



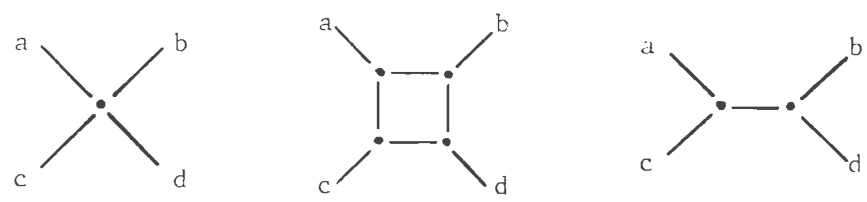
Edges

With non-polygonal forms the numbering of the united circuits must be unified. The smaller circuit retains its original numbering, including the uniting edge joined to the lower node. Then the numbering of the nodes or edges of the senior partners follows in sequence. Example:



(a) (b) (c)

Quadrivalent Vertices. Some organic molecules of considerable interest have one or more 4-valent nodes, needing special provisions in our scheme. The system so far developed can be most advantageously exploited by treating an n-valent node as the collapse of some subgraph on which n edges are afferent. Two possibilities for a 4-valent node (a) are 2.40

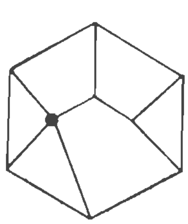


(a) (b) (c)

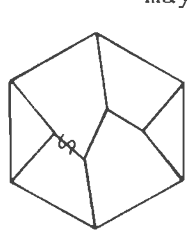
The second (c) has the advantage of adding only one virtual node per 4-valent center. Quadrivalent centers will therefore be treated as collapsed edges of a parental trivalent graph. The adjacent edges (abcd) can be divided in three different ways: ab/cd, ac/bd and ad/bc, hence there may be as much as a threefold ambiguity in the choice of parental graph. This will ordinarily be less on account of symmetry. 2.41

The ambiguity can be fully resolved by the following canons of choice of parent graph.

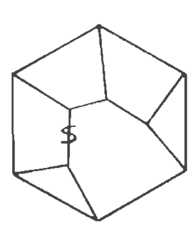
1. Avoid a separable graph. Hence  is related to  and not .
2. Avoid a gauche graph if possible.
3. Avoid a nonplanar graph if possible.
4. From the remaining possibilities, choose the graph which, in canonical form and listing, stands lowest. For an example, n = 9



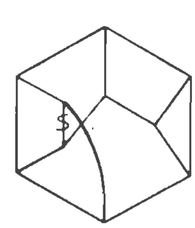
may go into



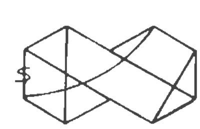
(a)
BCDDB



(b)
BCCCB



(c)
[GAUCHE]

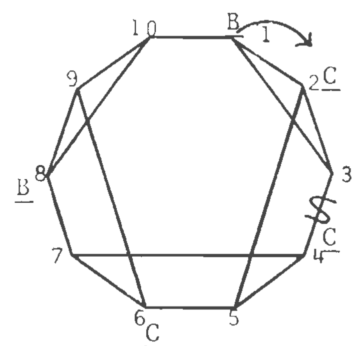


(c')

(a) and (b) are readily reduced to their canonical form. (c) is recognized as gauche (see the graph 6CCC as the left part of the isomorphic (c')-- the numbering of a Hamiltonian circuit is displayed to help along), and therefore disqualified. In the tables, (a) and (b) are already known as BCDDB and BCCCB respectively. By canon 4, the choice is BCCCB.

The encoding follows the principles for mapping other paths to be detailed in Part III. However, the specification of contracted edges (spiro fusions) is given at a separate, first level of priority , to bring structural homologues under a common heading. Where symmetries require a choice, the spiro fusions will be mapped on the edge list so as to maximize this vector. I.e., they are placed as early in the list as possible. The numbering of vertices and edges is retained as given in 2.3. That is, a virtual node remains in the list.

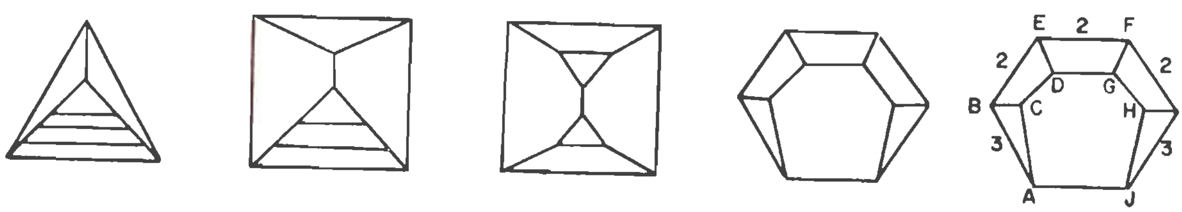
The present example becomes



i.e., the spiro fushion is mapped on the 3rd edge of the circuit. The coding is a reasonable one to mark the vertex group for these figures. Additional examples are summarized in Table 2T.7. Applications to complete graphs are detailed in Part III. The program contains a sufficient list of canonical forms and synonyms to expedite the translation of any vernacular input codes. These manipulations are not particularly difficult to program, but as already demonstrated can be quite tedious by hand.

Planar Mesh Representations. Besides the isometric perspective and polygonal representation, any polyhedron can be represented as a planar mesh. Consider the polyhedra projected on a sphere. Then choose any face for a base and expand it, flattening the rest of the sphere to an enclosed plane. This operation shows that any polyhedron has a planar representation (no edges crossing); furthermore, any distinct face will give a different appearance when expanded. Usually the largest face will give the most nearly conventional representation. When the mapping is expanded, this will usually be more nearly reminiscent of the usual structural formulas than the more abstract figures so far presented. 2.50

The isomorphic variants of planar meshes obtained by choosing alternative faces as the base (see Fig. 2.51) are generally very unfamiliar, pointing up the importance of a canonical representation. 2.51



ABC OR AIJ — 10A3

BCDE OR FGHI — 10A4A

DEFG — 10A4B

ABEFIJ OR ACDGHJ — 10A6

10A6 WITH MAPPING OF BENZOPERYLENE

Reconstruction of planar mesh from Hamilton circuit representations.

2.52

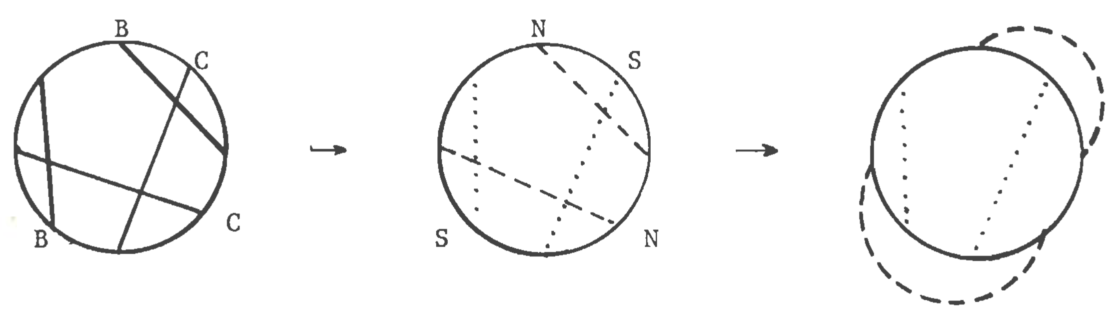
The polygonal representations of figure 2T.4 and 2T.5 are undoubtedly confusing owing to the intersection of chords belonging to different faces. A simple algorithm can help to resolve these figures; it is also useful for the computer reconstruction of planar maps, closer to the chemist's customary models, from the canonical codes. 2.53

The main idea is to regard the polygonal form as projected on a sphere, the polygon forming the equator. Then, for a planar map, the chords must be classified into two sets, one for each hemisphere. Within either hemisphere, no chords intersect. The visualization of these structures still requires some practised imagination, especially to avoid the identificaiton of the Hamilton circuit polygon with any face of the polyhedron. However, as any face will be bounded by edges from the cirucit and from one hemisphere, the marking of faces is facilitated for chemist and computer alike. In practice the computer should carry all the burden of these transformations. 2.54

The grouping of chords is quite simple. The assignment of N vs. S hemisphere is, of course, arbitrary; the first chord is assigned N. Then each succeeding chord is tested for intersection with the N set so far. If not, it is added to the N set. If it does intersect, it should be added to the S set. If it also intersects a chord already in the S set, the graph is non planar. Indeed this is the most effective algorithm for the purpose. 2.55

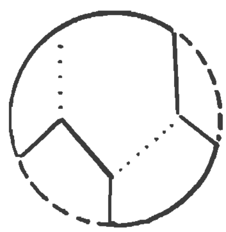
Planar meshes come directly from the chord groupings. The chords of one hemisphere are merely brought outside the polygon. Thus, for the pentagonal wedge,

BCCB 2.551

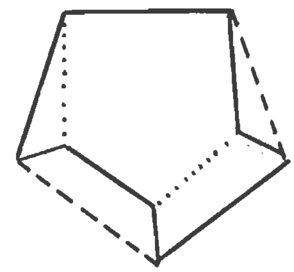


which takes only a topological deformation to yield

2.5-2

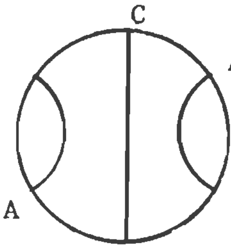


recognizable as

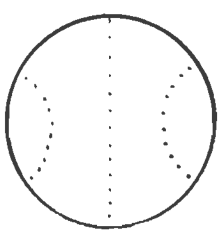


When the map is a 2-connected union an obvious ambiguity may arise, some chords intersecting with neither of the remaining sets. This does not impair the construction of a planar mesh.

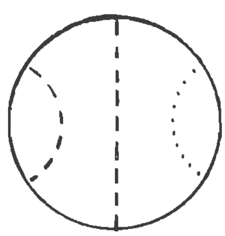
2.5-3



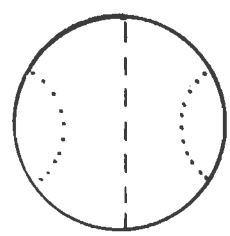
could be



or



or

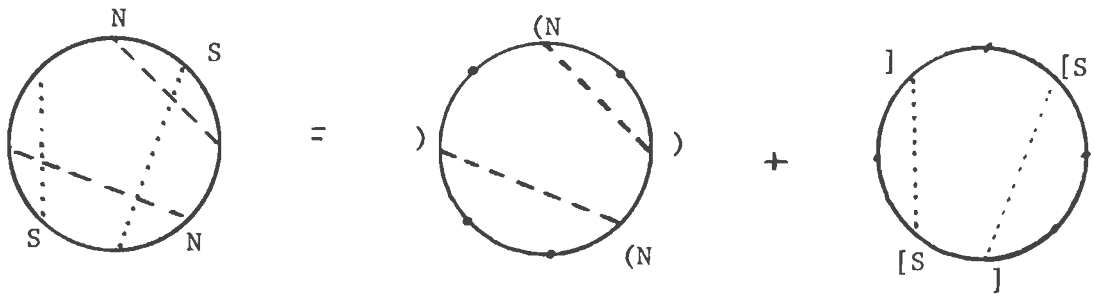


etc.

The rule would be: place a chord in the S hemisphere (inside) if it is ambiguous. This ambiguity is probably the main source of disparity in conventional chemical symbolism; related to it is the choice of face to circumscribe the map.

Nested parenthesis notation and combinatorial generator. 2.56

Since the chords of one hemisphere do not intersect, the labels that signify their start and end have the properties of nested parentheses, the matching of left and right parentheses being implicit in the description. For the two hemispheres 2.561 of BCCB we have



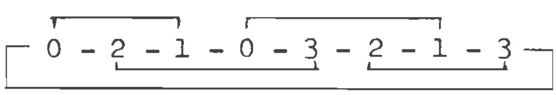
and superimposing the parentheses and brackets we have a descriptive formula

([)(][)]

This is economical in the computer program since it codes the signs as 2-bit numbers, the formula becoming

02103213.

Such a formula can be translated into a usable mesh diagram on sight:



It is also the basis of a rather more efficient generator program than the one mentioned in 2.232. Besides the economy of compact representation of the codes as quaternary numbers, it is easy to restrict the generator to minimize fruitless efforts with meaningless codes (e.g., extra right parentheses) and redundant forms (interconversion of () and []; some rotational symmetries). The notation is already explicitly limited to Hamiltonian planar maps. For certain investigations, additional restrictions like absence of triangles, cyclic connectedness at a level of at least 3 (i.e. polyhedra), 4, or 5, and other features can be rather easily added. However, the output is replete with isomorphisms, for which the technique of 2.232 is still the most efficient.

Further Developments in the Theory of Trivalent Graphs.

Polyhedra. **Since** the above material was composed and most of the computations run, some additional contributions in the literature have come to light. 2.60

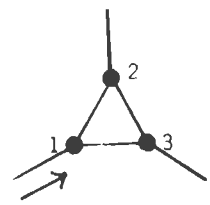
It was especially surprising that the enumeration of the polyhedra had not been worked out already in Euler's time or earlier, in view of classical 2.61
insight into the five regular polyhedra (of which three, the tetrahedron, the cube and the dodecahedron are included in our trivalent graphs, n_4, n_8, and n_{20} respectively. In 1900, however, Brückner[4] constructed the trivalent polyhedra for n up to 16, and we could confirm the equivalence of his set with the results of our computer programs through n = 12.

Little additional work has been done on this problem, except by Brückner. However (and independently of the present studies!) Grace has just published a 2.62
dissertation on the computation of the polyhedra through n = 18 (Grace, 1965). This work faces formidable problems in testing for isomorphism ($18! = 10^{15}$)-wise permutational searches being prohibitive. Mathematical theory evidently still lacks an analytical approach to this problem. Grace then used a conjectural criterion of isomorphism, "equisurroundedness". According to Grace "Equisurroundedness is a necessary but not a sufficient condition for isomorphism. The necessity is obvious...." He gives a counter-example with 17 faces to show the insufficiency. It is therefore uncertain whether he may have retained an incomplete list of polyhedra, as it is unknown whether some smaller polyhedra than with 17 faces may be equisurrounded with, but not isomorphic to, members of the list that has been retained. Grace did find some forms that Brückner had overlooked.

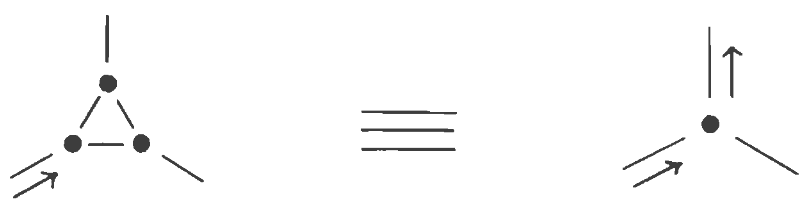
The polyhedra through n = 18 have been verified to have Hamilton circuits, including the classes n_{14}, n_{16}, and n_{18} as listed by Grace. It should be remarked 2.63
that the test for isomorphism (see 2.232) of polygonal graphs is relatively efficient, since << 2^n operations (contra n!) can establish (a) whether a graph has a Hamilton circuit and (b) if so, establish a canonical form for comparison with other graphs.

This test could be applied to Grace's for generating polyhedra program to discover any polyhedra smaller than n_{46} (Tutte's example) that might lack a Hamilton circuit, (see 2.230) and a more rigorous criterion of isomorphism than equisurroundedness can furnish.

The task of scrutinizing polyhedra for Hamilton circuits is simplified considerably by the reducibility of a triangular face. Consider a trace of a Hamilton circuit at its first incidence on a triangle: 2.64



Plainly if all 3 of its nodes are to be visited, it must be at this occasion. A path -1-2 without 3 would leave 3 stranded, i.e., would make a Hamilton circuit impossible. The complex -123- is therefore tantamount to a single node.



ORDER = N　　　　ORDER = (N-2)

Thus, if the (n) graph has a triangular face, and a Hamilton circuit, some (n-2) graph will likewise have a Hamilton circuit. Without formal proof, we assert that if (n) is a polyhedron, so is (n-2). 2.65

By induction we may then pass over (n)-polyhedra that have any triangular face, provided we have scrutinized all the (n-2) cases, which can be handled in part by the same process. As shown by the following table, this argument reduces the work for the polyhedra up to 18 vertices from 1555 down to only 55 cases.

2.66

N	Total Polyhedra	Non-triangle-containing Polyhedra
4	1	0
6	1	0
8	2	1
10	5	1
12	14	2
14	50	5
16	233	12
18	1249	34
Total n $\leq$ 18	1555	55

109

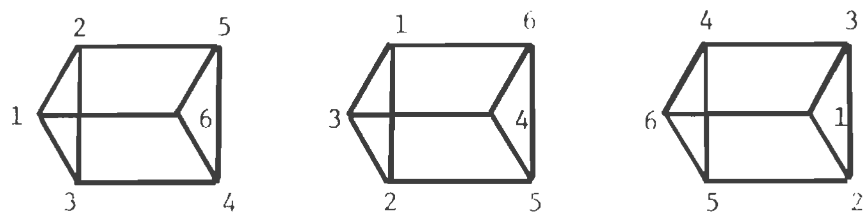
103

The listings of tables 2T.2 anticipate the polygonal graphs through 12 vertices, that is 8 faces, (or 7 rings within the meaning of the Ring Index). From Grace's work we can readily enlarge this anticipation to 18 vertices, (11
faces or 10 rings) but have not made the extensive enumerations called for. 2.6.7
The count of unions and particularly of gauche graphs increases even more rapidly than that of the polyhedra. On the other hand, the notational system will accommodate any polyhedron that has a Hamilton circuit, as well as unions of such polyhedra; such structures can be coded as they are defined without being anticipated in advance. The generator would then be confined to an empirical list of previously discovered forms. This may be a practical necessity for the highest order forms in any case, where the rapidly increasing number of possible arrangements contrasts with relatively few realizations.

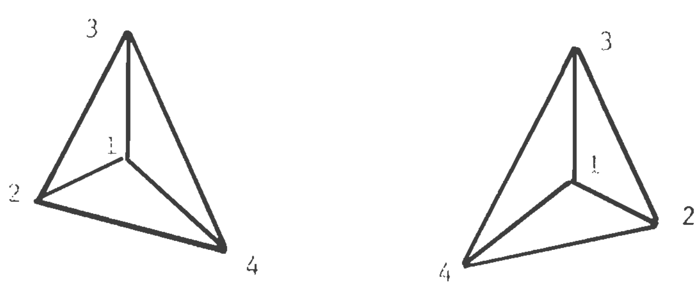
The most complex rings, in practice, are related to polyhexacyclic 2.6.8
hydrocarbons. This special class can be accommodated by another approach, elaborated in Part 6. This involves the mapping of the polyhexacycle on a selection of "tiles" from a continuous hexagonal tessellation or mosaic. An enumeration of these forms is also given in Part 6.

Symmetry classification.

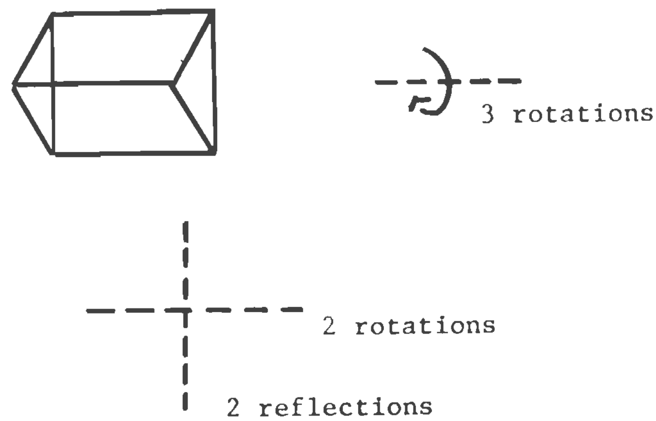
The symmetry of the vertex group plays a central role both in mapping known structures and in the generation of non-redundant lists of hypothetical structures. The essential problem is that the same topological relationship may have many alternative representations, which is to say that the diagram can be manipulated so that it is self-congruent. If the vertices are labelled, different sets of vertices will describe the same figure. E.g.,



Since we are dealing with topological groups, not rigid bodies, the symmetries carry even further, i.e. the tetrahedral cases are not distinguished (stereo-isomerism being dealt with at another level).



The polyhedral representations generally make the set of symmetries self-evident (which the planar ones sometimes do not). For example, the prism has 12 equivalents 2.701



while its Hamiltonian polygon  displays only 4.

Although not a profound task, the manual enumeration of the symmetries, say for table 2T.2, would be a tedious one and an algorithmic approach would be preferred. 2 702

One approach is to generate the whole symmetric group, S_n, the n! permutations of the vertex codes, and test each of these for congruence with the canonical form. But this is almost prohibitively costly for n = 10, as 10! = 3,628,800 trials, or probably about one minute of computer time per set.

Instead we can rely upon the set of Hamiltonian circuits, where they exist. Each symmetry operation will generate a corresponding representation of a Hamilton circuit. Consequently the set of symmetries will be included in the set of Hamilton circuits. These can be generated by a binary search of << 2^n trials, far less than the n! of the whole symmetric group. In fact this list of Hamilton circuits was saved from the initial computation of table 2T.2 for use as the input data of this calculation. 2 703

The algorithm can be summarized

1. <u>Take E as the canonical form from table</u> 2T.2. Convert the chord list to an **incidence** matrix (connection table) of the n vertices with one another.

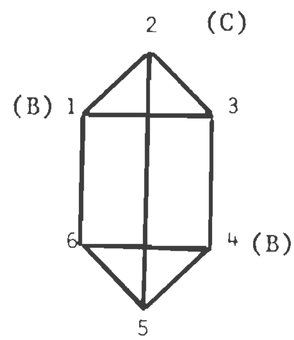
2. <u>Test E for its symmetry on the plane</u>. That is, test E under 1(1)n-1 steps of rotation of its indices [the permutation cycle $\begin{pmatrix}123...n\\234...1\end{pmatrix}$] before and after reflection, $\begin{pmatrix}123..n\\n..321\end{pmatrix}$. When the permuted incidence matrix becomes congruent with E, a symmetry operator is revealed. This set of operators is saved.

3. <u>Each Hamilton circuit is tested for potential congruence with E</u> under rotation and reflection. The isomorphisms (indicated in table 2T.2) cannot be made congruent to E and are rejected. The congruences are saved as equivalents under symmetry.

4. Each of these is also subjected to the operators found in step 2.

5. The list is sorted and redundancies are removed. This can also be done prior to 4 if the list is a long one.

6. The list now contains all of the symmetries expressed as permutations. Further classifications can be made, as indicated, on this list. For many purposes it can be used as is.



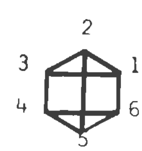
Example. Consider the prism, BCB

a. This is readily translated into

$\overline{123456}$ plus $\overline{13}$,$\overline{25}$ and $\overline{46}$.

b. E is of course 123456. The symmetries of rotation (C_2) and reflection (I) are readily found and give

123456 456123 654321 321654.



[321654]

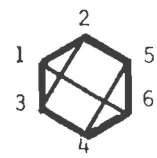
7. Our program gives the following additional Hamilton circuits. For efficiency, the search was initialized at vertex 1 and considered only the paths $\overline{12}$ and $\overline{13}$ as candidates for the first trial choice. That is, the rotation and reflection operations were anticipated. Hence the circuits as found are potentially, not actually, congruent with E. At this point they are

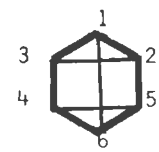
125643 134652 132546.

The first two require a rotation; the last is already congruent. When rectified we then have 312564

2.113

312564 213465 132546





8. These are used as operands under the operators found in 2. Together with E we then have

E	456123	654321	321654
312564	564312	465213	213465
213465	465213	564312	312564
132546	546132	645231	231645

9. After sorting and weeding out we have the 12 cases.

123456	213465	312564	456123	546132	645231
132546	321645	321654	465213	564312	654321

For small n of course we can more readily operate on a visual image of the prism at speeds that compare with the computer. But recording the results becomes a bottleneck in more extensive work.

General Systematics of Graphs. Composition of graphs from Hamilton Circuits: 2-connected graphs.

2.72

A more general approach to the description of circuit-free graphs has been devised based on the level of connectedness of the graph, i.e., the least number of cuts needed to separate the graph.

The cases of chemical interest are all 2-connected, and have already been discussed in section 2.262.

2.73

Canons of Analysis. A 2-connected graph found to be circuit-free is subjected to trial dissections of its bilineal unions, designed to show a construction under the following criteria. The principle of analysis is to obtain a dissection of the graph into

1. *A minimum number of circuits*
2. *At the lowest level of connectedness.*

In effect, the dissection maps the *circuits* of the graph on to the *nodes* of a "hypergraph." If a Hamilton circuit is present this hypergraph consists of a single node. Otherwise it may be a node-pair (i.e. a pairwise union of circuits) or in principle a more complex tree or even a generalized connected graph. The hypergraph is then evaluated according to the same principles as laid out for chemical graphs -- the *nodes* being the *circuits*; the *edges* being the *sets* of circuit-joining edges. We can therefore add the criterion:

3. *Giving the maximum valued hypergraph.*

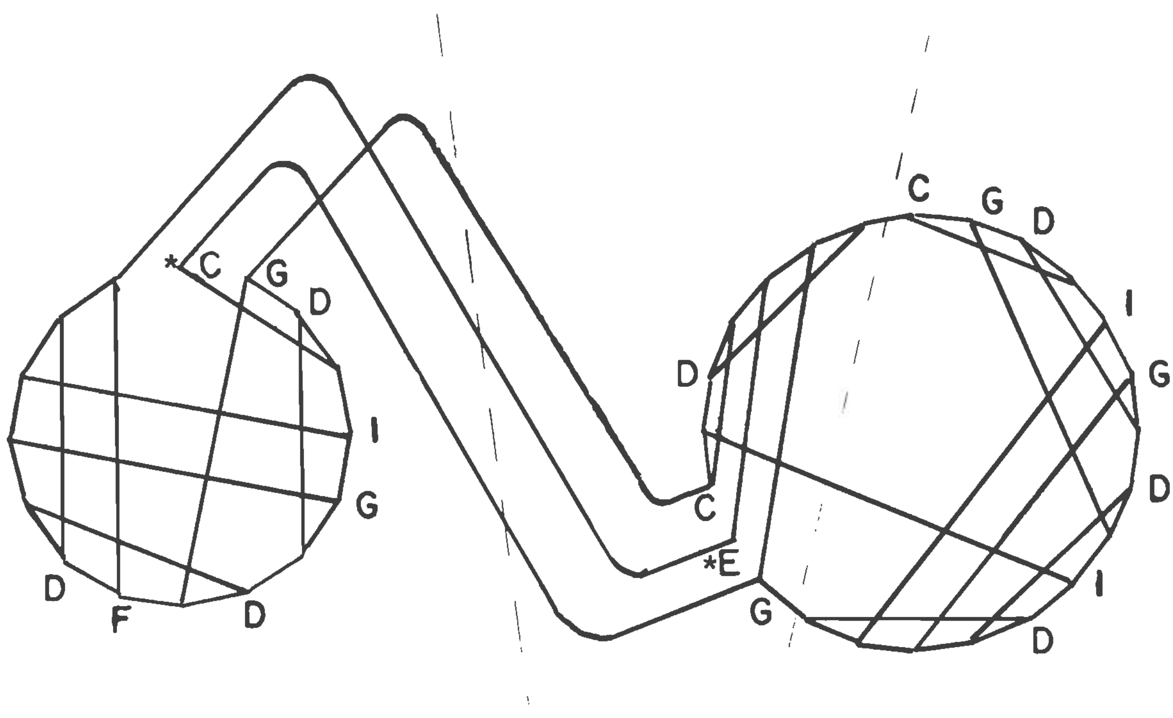
The evaluation of the hypergraph may entail searching its set of circuits, as may be done recursively to any depth.

This analysis leads to some predictively useful principles concerning the occurrence of non-Hamilton graphs. A given circuitable graph is readily analyzed for the presence of three kinds of edges (1) the most usual edges participate in some but not every circuit (2) "must-edges" participate in every circuit, or (3) "non-edges" participate in no circuit. 2.74

A bilineal union in which a non-edge of either or both component graphs is spliced then forms an HC-free graph. 2.75

The same approach can be used for 3-connected graphs. In this case, a 3-cut residue is obtained by extracting one node from a graph. If one of the cut edges is a must-edge, it will retain this property in its compositions. Thus, in Tutte's example, replacing 3 nodes of a tetrahedron by a 15-node residue with a must-edge results in a 46-node circuit-free graph. (Fig. 2.23). 2.76

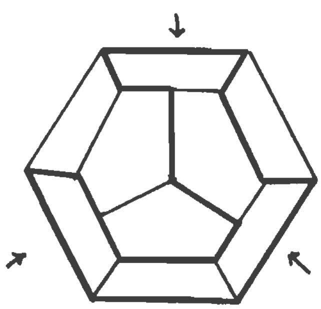
There is no present compulsion to rigidify the notation for such complex graphs; one suggestion is implicit in the diagram:



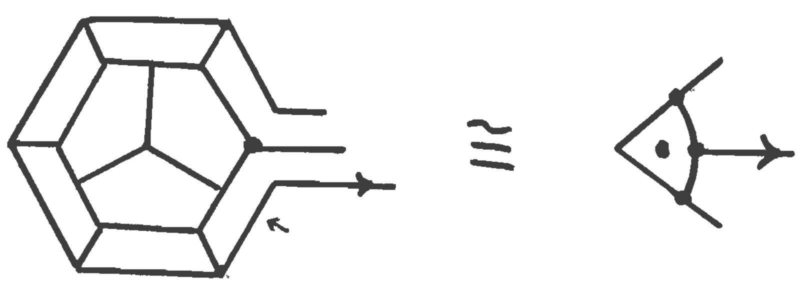
(38CGDIGDIDGE*CD:231:C*DIGDFD)

This 38-node graph is the same as 2.78d; the polygons are oriented in canonical form. The *'s signify the extracted notes whose removal leaves the 3-cut graphs; the 231 specifies the splicing of the cut edges. Note that the subgraphs to the right and left of the dashed lines are the same. The construction shown follows the rule of dissection into maximum 3-connected circuits.

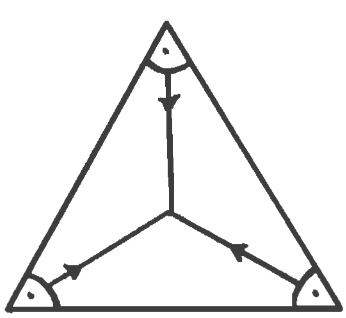
This graph which is the same as 2.78d is almost certainly the smallest non-Hamiltonian polyhedron; it is known to be the smallest which is cyclically 3-connected. All candidate graphs $n \leq 24$ have been explicitly examined. Its construction may be clarified by noting the must-edge (marked by arrow in 2.78a). A residual 3-cut graph can be planted, as shown, in 2.78c and 2.78d in configurations inconsistent with must-edges in these figures. 2.78c is Tutte's 46-node graph, already figured at 2.23. The dashed lines on 2.78d correspond to those on 2.77. 2.78



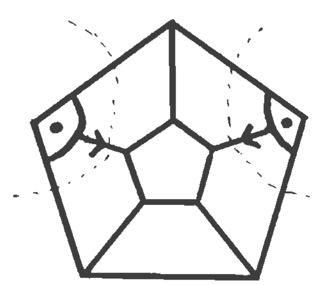
(a)



(b)



(c)



(d)

Coding and Reconstruction of Hamilton Circuits

Each graph is represented as a Hamilton circuit projected on the boundary of a regular polygon with n vertices. Joining these n vertices are $\frac{n}{2}$ chords, since each vertex is trivalent. The locations of these chords are specified by $\frac{n}{2}$ characters, integers being replaced by the alphabet to obviate punctuation*.

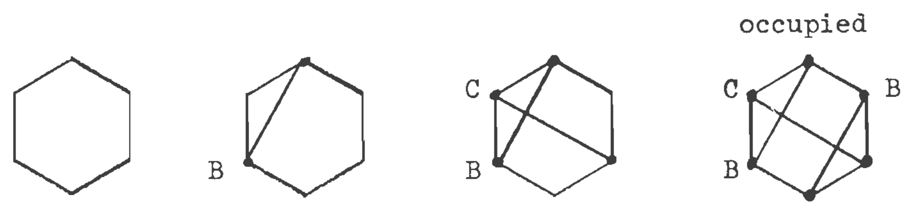
To reconstruct the graph:

1) Draw the n-gon

2) Start at an arbitrary node and draw a chord whose span corresponds to the first character

3) For each successive character, move to the next unoccupied node.

Hence, the steps for 6BCB are:



6 6B 6BC 6BCB

* A	1	F	6	K	11	P	16	U	21
B	2	G	7	L	12	Q	17	V	22
C	3	H	8	M	13	R	18	W	23
D	4	I	9	N	14	S	19	X	24
E	5	J	10	O	15	T	20	Y	25

Appendix:

Algorithm for finding Hamilton circuits of a cyclic graph.

This is illustrated for an undirected, trihedral graph but should be generalized without difficulty in an obvious way. The input is a description of the connectivity of the graph. The essence of the routine is to build a table of sets of edges so that just two edges incident on each node appear in any row of the table. The first node is chosen arbitrarily. Its three incident edges are marked <u>current</u> and <u>open.</u> The circuit-fragment table is started with three rows by listing the 3 pairwise choices among the current edges.

1. Select an open edge. The two adjacent edges become the trial edges.
2. How many trial edges match the current list: none, one, or two?
    a. If none match, close the selected edge and replace it on the current open list by the two trial edges. Scan the circuit-fragment table. Each row in which the selected edge appears is replaced by two rows, one for each trial edge. Each remaining row is replaced by one row showing both trial edges. Go to 1.
    b. If one matches, a circuit of the graph has been closed. Scan the circuit-fragment (c.f.) table contrasting the matched edge with the selected edge. Each c.f. where neither appears is deleted. If one of the two appears on a c.f., this is augmented by the trial edge. If both appear, the c.f. row stands as is unless a tracing of the c.f. shows it to be prematurely closed, whereupon it is deleted. Go to 1.

c. If both match two adjacent faces of the graph have been closed. The preceding subroutine is revised in an obvious way to close out both matched edges: those c. f. rows are retained which are compatible with the indicated edge allocations. Go to 1.

The process is terminated when the open edge list is vacated. If 2.91
this leaves some nodes unused, no Hamilton circuit is possible. Otherwise, the final closure of circuit-fragments leaves a table of circuits. This must still be scanned to separate the Hamiltonian circuits from the set of pairwise disjoint circuits.

The efficiency of the algorithm depends on keeping the current c. f. 2.92
table as small as possible. This is accomplished by a lookahead routine which scans prospective choices of current edges to seek the promptest closure of a face.

For an example, Tutte's 46 node non-Hamiltonian graph has been searched 2.93
exhaustively. This required a c. f. table of 12,477 rows consuming 29 seconds of a program on IBM 7090. Searches yielding all the circuits of other large Hamiltonian graphs required a comparable effort.

This procedure may have some utility for studies on classification, 2.94
isomorphisms, and symmetries of abstract graphs and other network problems for which the set of Hamilton circuits is often an advantageous approach. A complete description of the computer program is available from the author.

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1. Tait, P. G., Phil. Mag. (Series 5), 17: 30 (1884).

2. Tutte, W. T., J. London Math. Soc., 21: 98 (1946). (See also reference 3)

3. Tute, W. T., Acta Math. (Hung.), 11: 371 (1960).

4. Brückner, M: Vielecke und Vielfläche. Teubner, Leipzig, 1900.

5. Grace, D. W., Computer Search for Non-Isomorphic Convex Polyhedra, Stanford Computation Center Technical Report No. CS15 (1965).

PART II. GENERAL TABLES.

2T.1	Count of cyclic trivalent graphs.
2T.2	Symbolic listing of cyclic trivalent graphs $n \leq 12$ and polyhedra $n = 14$.
2T.3	(Deleted)
2T.4	Nonpolygonal cyclic trivalent graphs $n \leq 12$.
2T.5	Figures for graphs $n \leq 12$ with chemical examples.
2T.6	Figures for polyhedra $n \geq 14$ which have chemical examples.
2T.7	Quadri-trivalent graphs.

COUNT OF CYCLIC TRIVALENT GRAPHS

[and genera of known chemical graphs]

Vertices	Number of Chemical Rings+	With Hamilton Circuits: Polyhedra	With Hamilton Circuits: Unions (Planar)	With Hamilton Circuits: Gauche Forms (Non-Planar)	Without Hamilton Circuits: Planar Unions
0	1	1*	0	0	0
2	2	1*	0	0	0
4	3	1*	1*	0	0
6	4	1*	3*	1[0]	0
8	5	2*	10 [9]	3[0]	1*
10	6	5 [4]	37 [20]	18[0]	5 [2]
12	7	14 [3]	183 [35]	133[0]	30 [7]
14	8	50 [3]	[45]		[11]
16	9	233[3] [2]	[46]		[10]
18	10	1249[3] [5]	[25]		[5]
20	11	[1]	[21]		[4]
22	12	[1]	[6]		[1]
24	13	[2]	[9]		[1]
≥ 26	≥ 14	[0]	[14]		[3]

[Numbers in brackets are the count of genera of known examples from the Ring Index.] * signifies all.
Spiro forms are excluded from this count.

1 Figures drawn herewith.
2 Listed herewith
3 According to Grace (1965).
+ This is one less than the number of faces of a polyhedron.

2T.2 SYMBOLIC LISTING OF CYCLIC TRIVALENT GRAPHS.

<u>Polygonal Forms</u>: [Planar (polyhedral, unions), Nonplanar]

2T.20	n = 4, 6, 8	
2T.21	n = 10	
2T.22	n = 12	Planar polyhedra and unions
2T.23	n = 12	Nonplanar forms
2T.24	n = 14	Polyhedra only (with Grace [1965] catalog number)

<u>Nonpolygonal Forms</u>:

2T.25	n = 8, 10, 12	Summary table,(see 2T.4).

The canonical form is shown first on each line. Isomorphs (unrelated by rotation or reflection) are then shown. See 2T.254 for coding.

POLYGONAL GRAPHS

4 VERTICES

POLYHEDRON

4A	BB

PLANAR UNION

4B	AA

6 VERTICES

POLYHEDRON

6A	BCB

PLANAR UNIONS

6B	AAA
6C	ABB
6D	ACA

GAUCHE GRAPH

6X	CCC

8 VERTICES

POLYHEDRA

8A	BCCB	BDDB
8B	CECC	

PLANAR UNIONS

8C	AAAA
8D	AABB
8E	AACA
8F	ABCB
8G	ABDA
8H	ACDB
8I	ADDA
8J	AEBB
8K	AECA
8L	BBBB

GAUCHE GRAPHS

ACCC	
BDCC	
CDDC	DDDD

10 VERTEX GRAPHS

POLYHEDRA

BCCCB BEFDB
BCDDB BCEEC
BDEBB
BDECC
CFDEC

PLANAR UNIONS

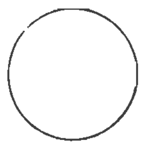
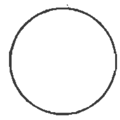
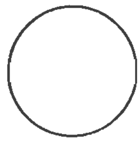
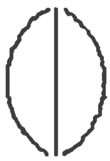
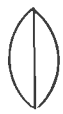
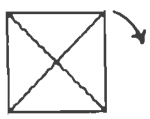
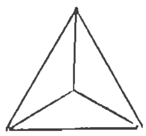
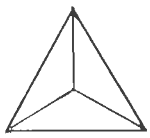
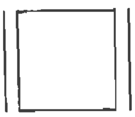
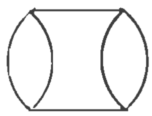
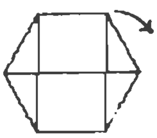
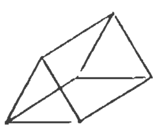
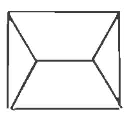
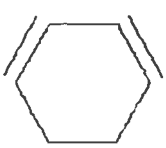
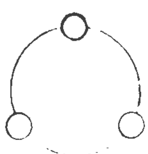
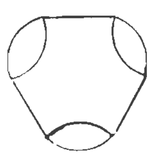
AAAAA
AAABB
AAACA
AABCB
AABDA
AACDB
AADDA
AAEAA
AAEBB
AAECA
ABBBB
ABBCA
ABCCB
ABCDA
ABDDB ABEBC
ABEAB
ABEDA
ABFBB

ABFCA
ACACA
ACECC AECEC
ACFCB ADFDB
ACFDA
ADADA
ADBEA
AEBEB
AFCEB
AFDEA
AFFBB
AGBCB
AGCDB
AGDCA
AGEBB
AGECA
BBBCB
BBCDB
BBEBB

GAUCHE GRAPHS

AACCC
ABDCC
ACCEA
ACDDC ADDDD ADDEC
ACDEB ADEEB
ACEEA AEEEA
ADECD
ADFCC
AGCCC
BBCCC
BCDCC BEFCC
BDCDB BEEEB
BDDDC BEDDD BEDEC
BDDEB
CCECC
CDEDC DFDED
CEEDD CFDDD CGDCD DEEED
CEEEC CGCCC EEEEE

GRAPHS OF POLYGONS OF ORDERS 0 - 6

POLYGONAL REPRESENTATION	POLYHEDRAL FORM	PLANAR MESH DIAGRAM	SPAN LIST
 —			—
 A			11
 BB			2222
 AA			1313
 BCB			234234
 AAA			151515

AND POLYHEDRA OF ORDER 8

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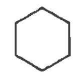
<tr><td>—</td><td>—</td><td></td><td>292</td></tr>
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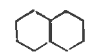
12</td><td></td><td>1754</td></tr>
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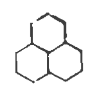
34 34</td><td></td><td>3620</td></tr>
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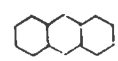
34 24</td><td></td><td>3618</td></tr>
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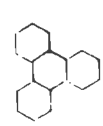
34 61 56</td><td></td><td>5256</td></tr>
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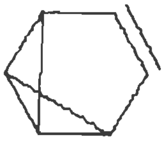
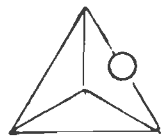
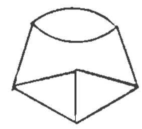
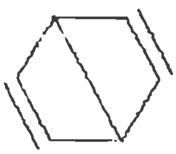
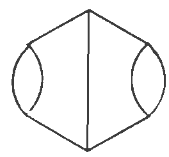
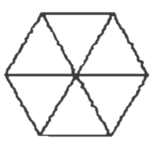
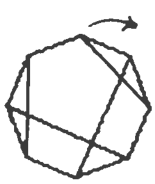
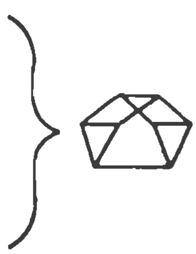
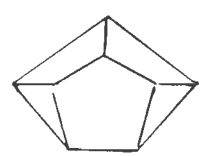
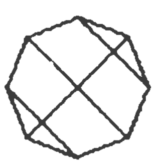
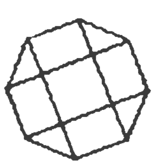
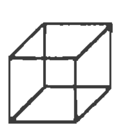
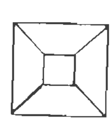
POLYGONAL REPRESENTATION	POLYHEDRAL FORM	PLANAR MESH DIAGRAM	SPAN LIST
 ABB			152244
 ACA			153153
 CCC	GAUCHE		333333
 BCCB			23635256
 BDDB			24642464
 CECC		 CUBANE	35353535

INCIDENCE MATRIX	CHORD LIST	EXAMPLE	RRI NUMBER OF EXAMPLE

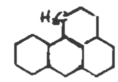
Incidence matrix

	2	3	4	5	6
1	2				1
2		1			
3			1	1	
4				1	1
5					1

Chord list

12	45	12
23	56	35
34	61	46

Example



RRI number of example: 5257

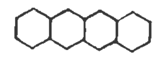
Incidence matrix

	2	3	4	5	6
1	2				1
2		1			
3			1		1
4				2	
5					1

Chord list

12	45	12
23	56	36
34	61	45

Example



RRI number of example: 5252

Incidence matrix

	2	3	4	5	6
1	1		1		1
2		1		1	
3			1		1
4				1	
5					1

Chord list

12	45	14
23	56	25
34	61	36

Example: NO EXAMPLE

RRI number of example: --

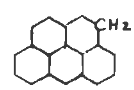
Incidence matrix

	2	3	4	5	6	7	8
1	1	1					1
2		1		1			
3			1				
4				1		1	
5					1		
6						1	1
7							1

Chord list

12	56	13
23	67	25
34	78	47
45	81	68

Example



RRI number of example: 6402

Incidence matrix

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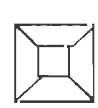
2		1				1	
3			1		1		
4				1			
5					1		1
6						1	
7							1

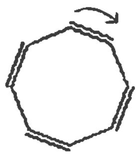
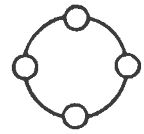
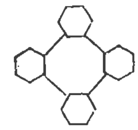
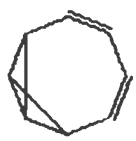
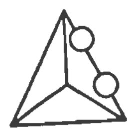
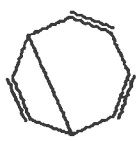
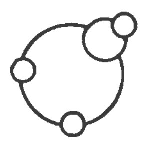
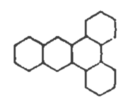
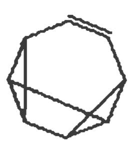
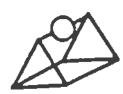
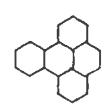
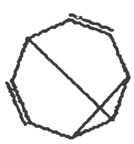
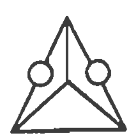
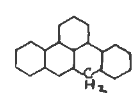
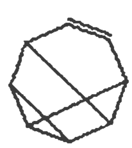
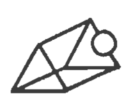
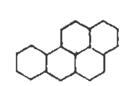
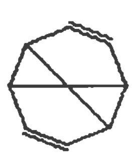
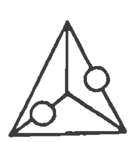
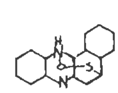
Chord list

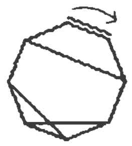
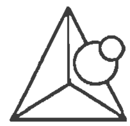
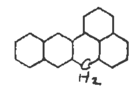
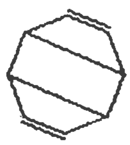
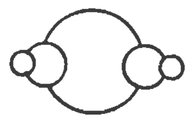
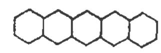
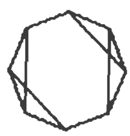
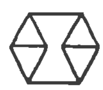
12	56	14
23	67	27
34	78	36
45	81	58

Example

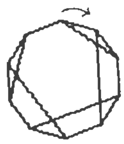
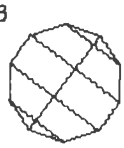
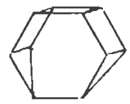
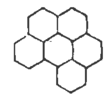
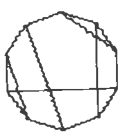
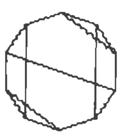
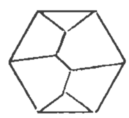
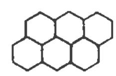
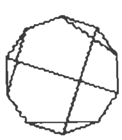
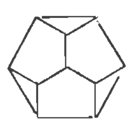
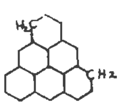
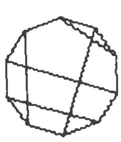
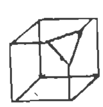
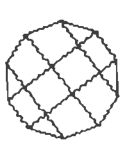
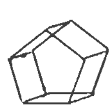


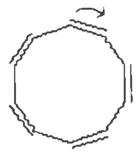
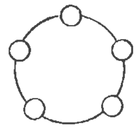
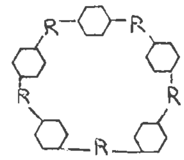
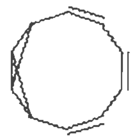
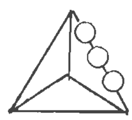
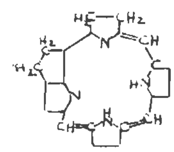
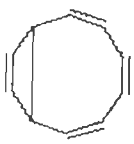
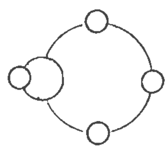
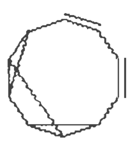
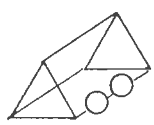
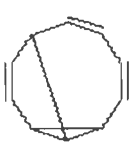
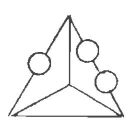
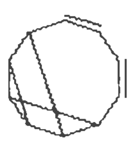
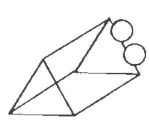
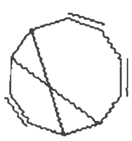
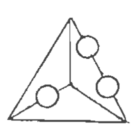
UNIONS OF 8 VERTICES

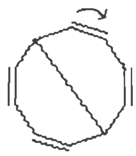
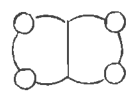
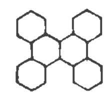
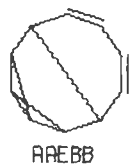
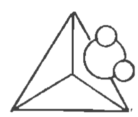
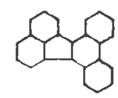
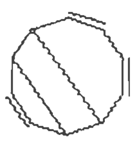
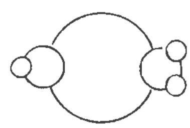
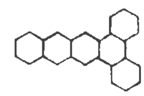
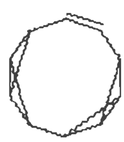
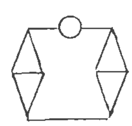
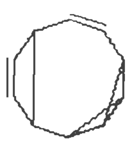
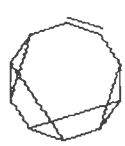
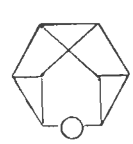
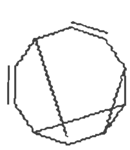
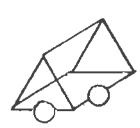
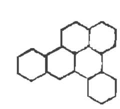
POLYGONAL REPRESENTATION	POLYHEDRAL FORM	EXAMPLE	RRI NUMBER OF EXAMPLE
 AAAA			6452
 AABB			
 AACA			6381
 ABCB			6400
 ABDA			6389
 ACDB			6399
 ADDA			6415

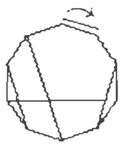
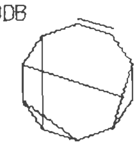
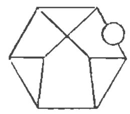
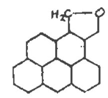
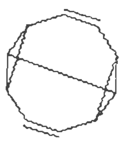
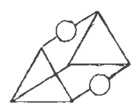
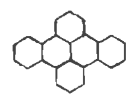
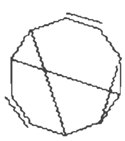
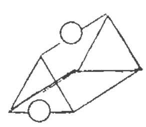
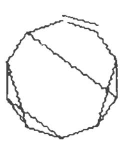
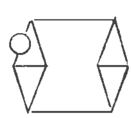
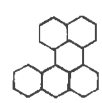
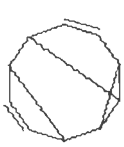
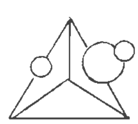
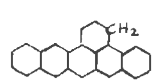
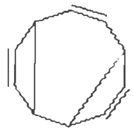
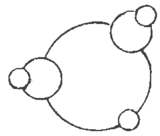
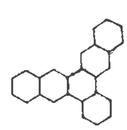
POLYGONAL REPRESENTATION	POLYHEDRAL FORM	EXAMPLE	RRI NUMBER OF EXAMPLE
 AEBB			6388
 AECA			6376
 BBBB			6401

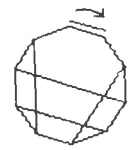
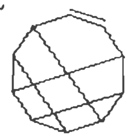
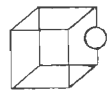
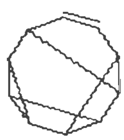
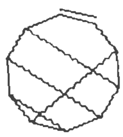
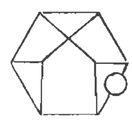
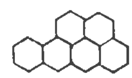
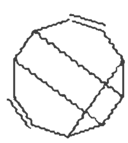
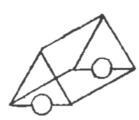
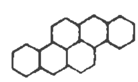
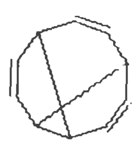
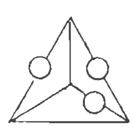
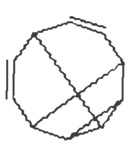
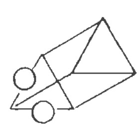
TRIVALENT POLYGONS OF 10 VERTICES

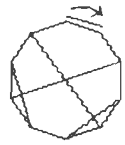
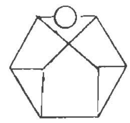
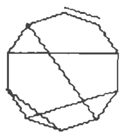
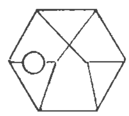
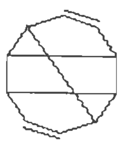
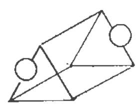
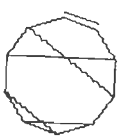
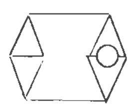
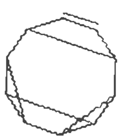
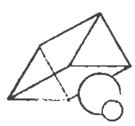
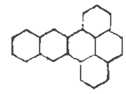
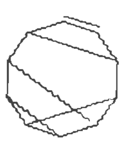
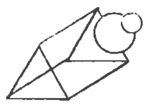
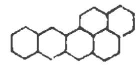
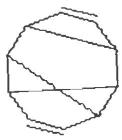
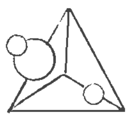
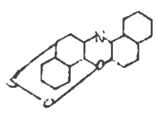
POLYGONAL REPRESENTATION	POLYHEDRAL FORM	EXAMPLE	RRI NUMBER OF EXAMPLE
 BCCCB  BEFDB			7036
 BCDDB  BCEBC			7033
 BDEBB			7034
 BDECC			
 CFDEC			6550

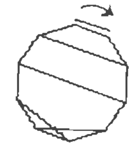
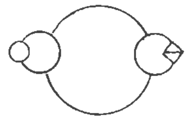
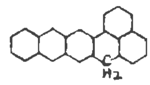
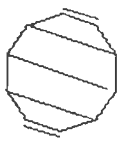
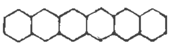
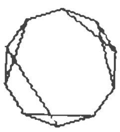
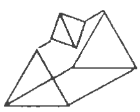
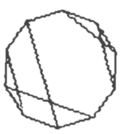
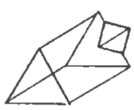
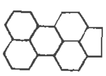
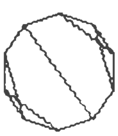
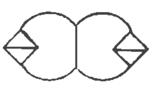
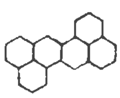
POLYGONAL REPRESENTATION	POLYHEDRAL FORM	EXAMPLE	RRI NUMBER OF EXAMPLE
 AAAAA		 $R = -(CH_2OCH_2)_2-$	9537
 AAABB			6561
 AAACA			
 AABCB			
 AABDA			
 AACDB			
 AADDA			

POLYGONAL REPRESENTATION	POLYHEDRAL FORM	EXAMPLE	RRI NUMBER OF EXAMPLE
 AAEAA			7010
 AAEBB			6852
 AAECA			6999
 ABBBB			
 ABBCA			
 ABCCB			
 ABCDA			7026

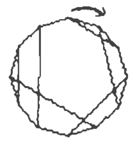
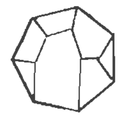
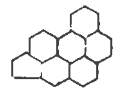
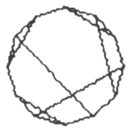
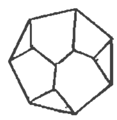
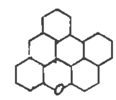
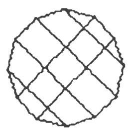
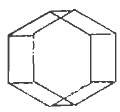
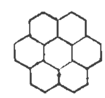
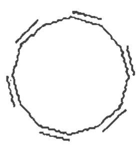
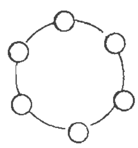
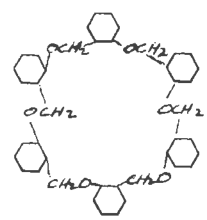
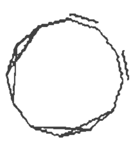
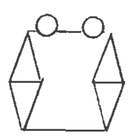
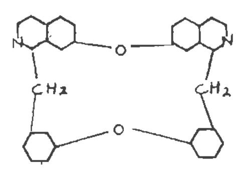
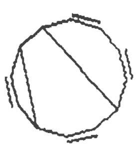
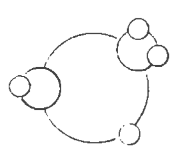
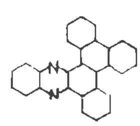
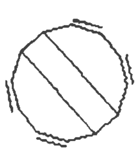
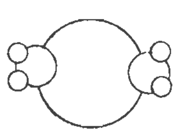
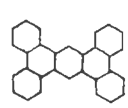
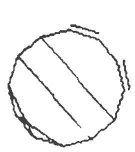
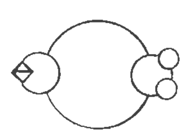
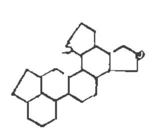
POLYGONAL REPRESENTATION	POLYHEDRAL FORM	EXAMPLE	RRI NUMBER OF EXAMPLE
 ABDDB  ABEBC			6782
 ABEAB			7022
 ABEDA			
 ABFBB			7023
 ABFCA			7015
 ACACA			7006

POLYGONAL REPRESENTATION	POLYHEDRAL FORM	EXAMPLE	RRI NUMBER OF EXAMPLE
 ACECC  AECEC			
 ACFCB  ADFDB			7031
 ACFDA			7028
 ADADA			
 ADBEA			

POLYGONAL REPRESENTATION	POLYHEDRAL FORM	EXAMPLE	RRI NUMBER OF EXAMPLE
 AEBEB			
 AFCEB			
 AFDEA			
 AFFBB			
 AGBCB			7021
 AGCDB			7020
 AGDDA			7042

POLYGONAL REPRESENTATION	POLYHEDRAL FORM	EXAMPLE	RRI NUMBER OF EXAMPLE
 AGEBB			7014
 AGECA			6996
 BBBCB			
 BBCDB			6863
 BBEBB			7025

POLYGONS OF 12 VERTICES WITH EXAMPLES

POLYGON	POLYHEDRON	EXAMPLE	RRI NUMBER OF EXAMPLE
 BCCDDB			7233
 BCDEBB			7341
 CGEGEC			7392
 AAAAAA			7411
 AABBBB			7409
 AAGACA			7271
 AAGEAA			7369
 AAGEBB			7120

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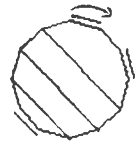
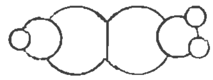
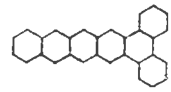
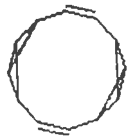
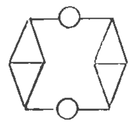
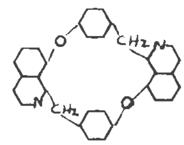
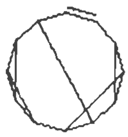
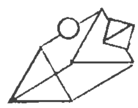
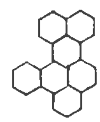
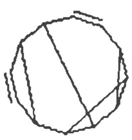
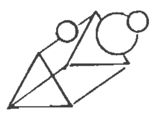
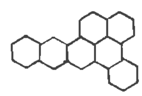
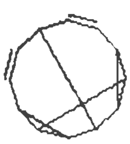
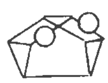
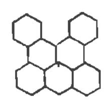
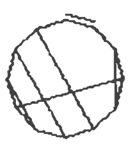
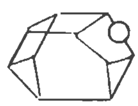
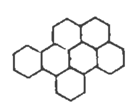
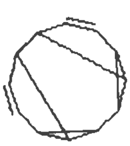
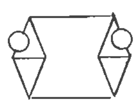
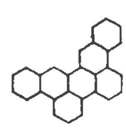
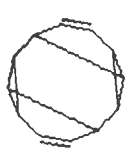
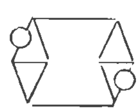
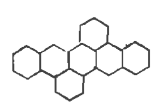
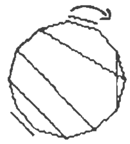
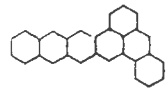
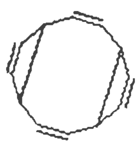
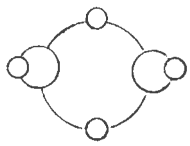
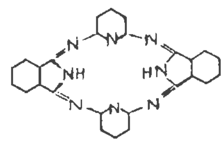
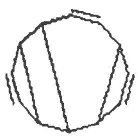
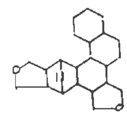
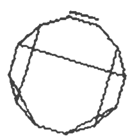
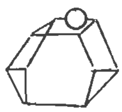
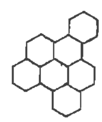
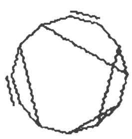
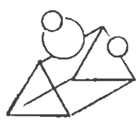
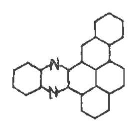
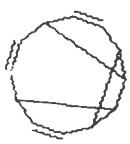
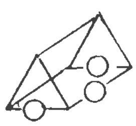
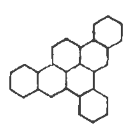
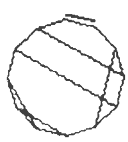
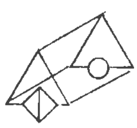
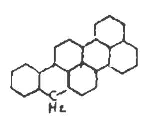
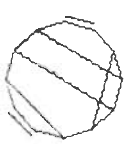
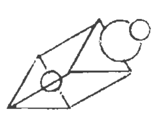
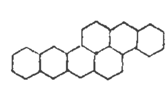
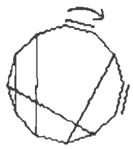
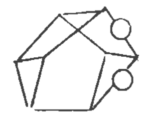
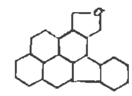
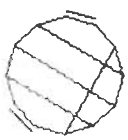
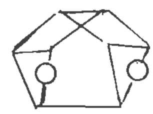
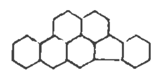
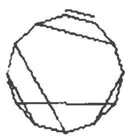
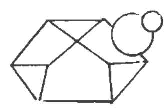
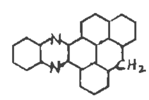
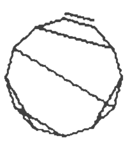
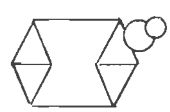
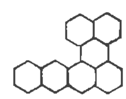
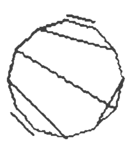
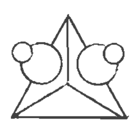
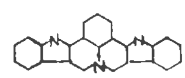
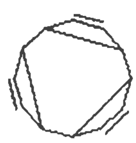
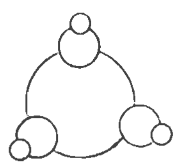
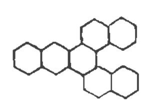
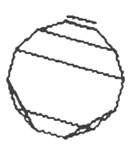
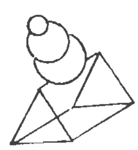
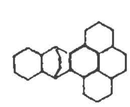
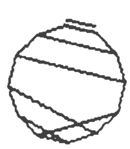
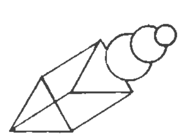
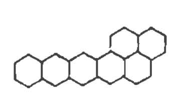
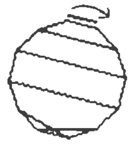
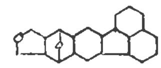
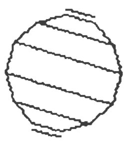
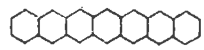
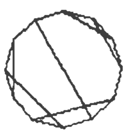
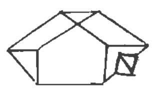
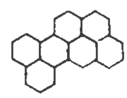
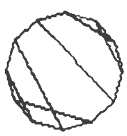
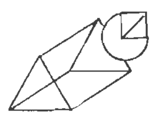
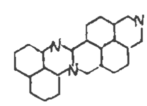
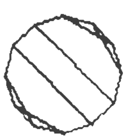
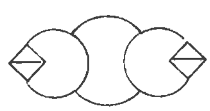
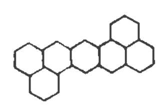
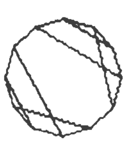
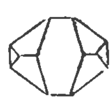
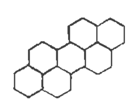
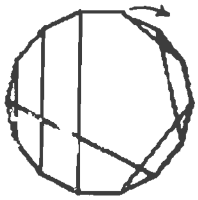
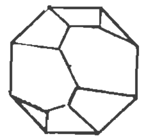
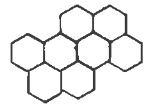
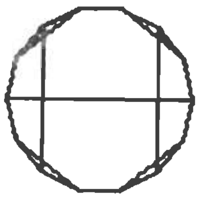
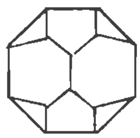
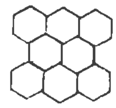
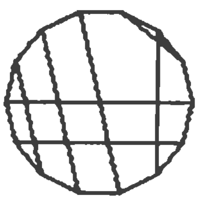
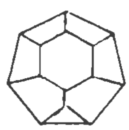
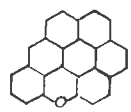
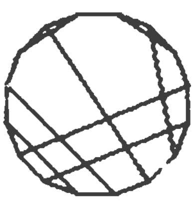
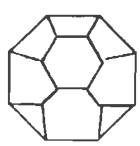
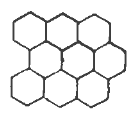
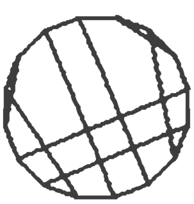
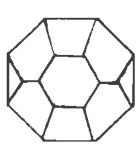
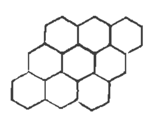
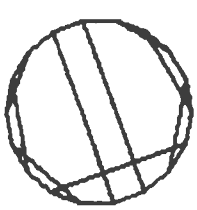
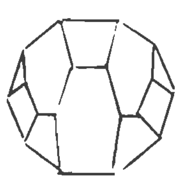
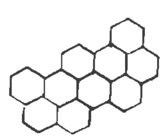
 AAGECA			7358
 ABBABB			7407
 ABCFBB			7388
 ABCFCA			7373
 ABDFBA			7389
 ABEFDB			7390
 ABHBDA			7378
 ABHDAB			7375

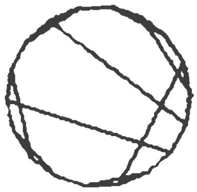
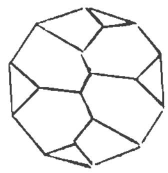
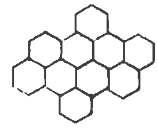
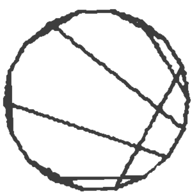
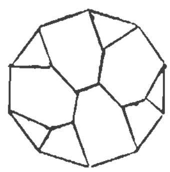
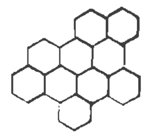
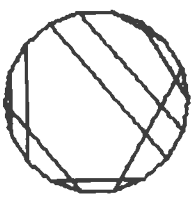
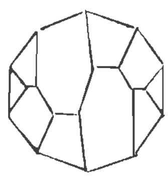
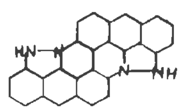
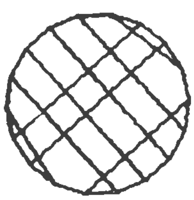
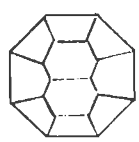
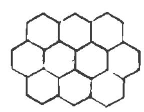
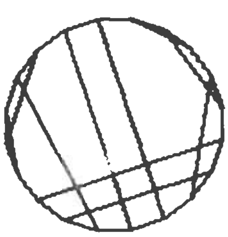
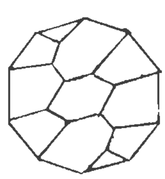
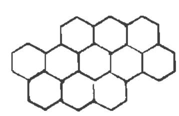
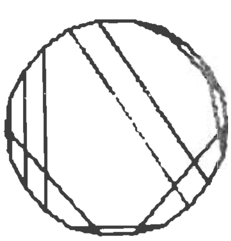
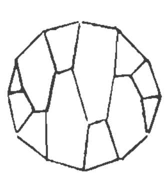
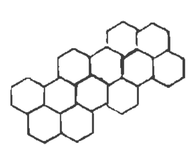
POLYGON	POLYHEDRON	EXAMPLE	RRI NUMBER OF EXAMPLE
 ABHECA			7370
 ACAACA			7174
 ACAECA			7146
 ACGBBC			9606
 ACHBCA			7277
 ACHDAA			7381
 ACHFBB			7387
 ACHFCA			7372

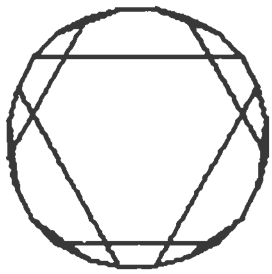
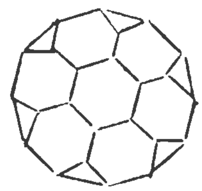
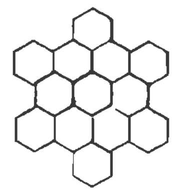
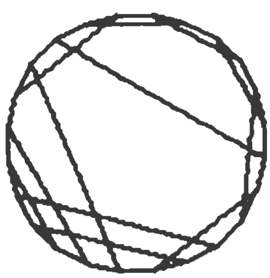
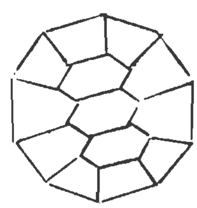
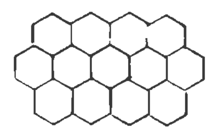
POLYGON	POLYHEDRON	EXAMPLE	RRI NUMBER OF EXAMPLE
 AOADDB			9558
 ADHFDA			7230
 AIBDDB			7276
 AIBFBB			7379
 AIBFCA			7136
 AICACA			7367
 AIGBCB			7396
 AIGCDB			9601

POLYGON	POLYHEDRON	EXAMPLE	RRI NUMBER OF EXAMPLE
 AIGEBB			7097
 AIGECA			7355
 BBCFCB			9602
 BBGCDB			9585
 BBGEBB			7376
 BCHCDB			7391

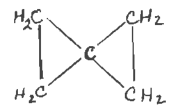
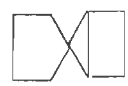
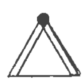
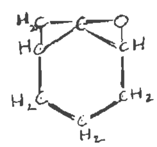
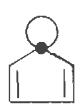
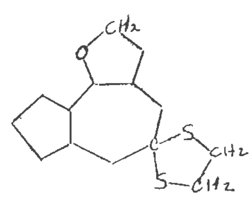
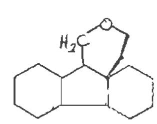
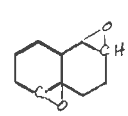
POLYHEDRA OF ORDERS 14-24 FOR WHICH CHEMICAL GRAPHS ARE KNOWN

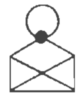
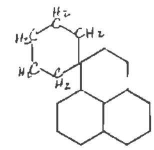
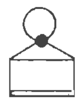
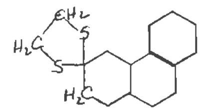
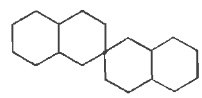
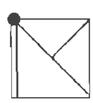
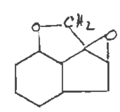
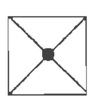
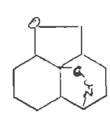
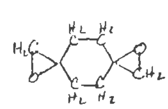
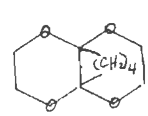
POLYGONAL REPRESENTATION	POLYHEDRAL FORM	EXAMPLE	RRI NUMBER OF EXAMPLE
 14 BCCEFDB			9652
 14 BDGBBDB			7529
 14 BDGEGEC			7511
 16 BDGEHECB			7623
 16 BDGEIGDB			7622
 18 BCCEJHCCB			9706

POLYGONAL REPRESENTATION	POLYHEDRAL FORM	EXAMPLE	RRI NUMBER OF EXAMPLE
 18 BCEKGBBCB			11505
 18 BCEKGCBBB			11506
 18 BCELJCDDB			7636
 18 CKIELJHFC			7653
 20 BCDGEKIFBC			7692
 22 BCCENLCEFDB			9725

POLYGONAL REPRESENTATION	POLYHEDRAL FORM	EXAMPLE	RRI NUMBER OF EXAMPLE
 24 BEQGBBEGBBEB			9733
 24 CUCDODGEHECD			9732

QUADRI/TRIVALENT GRAPHS DERIVED FROM TRIVALENT GRAPHS, n ≤ 8

CODE	GRAPH	EXAMPLE	RRI #
($1AA)			655
($3ACA)			2035
($3BCB)			2030
($5AACA)			8777
($5ABCB)			8964
($5ACDB)			3948

CODE	GRAPH	EXAMPLE	RRI #
($5AEBB)			5272
($A:5AECA)			4482
($B:5AECA)			5273
($5BCCB)			3966
($5CECC)			4615
($$2AECA)			2029
($$2CECC)			3418