

A Systematic Study of Symmetry Properties of Graphs I. Petersen Graph*

M. Randić

Ames Laboratory-USDOE, Iowa State University, Ames, Iowa 50011, U.S.A.

Received December 12, 1976

Recently (*Chem. Phys. Lett.* **42** 283 (1976)) a simple procedure for deriving symmetry properties of graphs has been suggested. It is based on a canonical numbering of the vertices of a graph, and consists in searching for all the acceptable numberings which have a unique adjacency matrix. In the series of papers initiated here we will apply the above procedure and derive all symmetry operations for graphs of interest to chemistry. We start with the Petersen graph which is of interest in discussions of isomerizations of trigonal bipyramidal structures.

INTRODUCTION

The importance of symmetry in physics and chemistry is for some time non generally accepted. The spherical symmetry of atoms and the point group for molecules arise in various problems and at a very elementary level in the study of molecular structure. The study of molecules with internal rotation by Howard¹ and later by E. Bright Wilson and collaborators² has shown that the effective molecular symmetry which dictates the selection rules in infrared and microwave spectra may be different from the symmetry of a rigid molecular frame. Hougen³ and Longuet-Higgins⁴ developed the topic of symmetry groups for such non-rigid molecules. These more general molecular symmetry groups are special subgroups of the full permutational group. They differ from the more familiar molecular point groups in having additional symmetry operations that are legitimate under somewhat relaxed constraints on the molecular geometry in these molecules with a relatively low barrier to internal rotations and inversions. Use of graphs in the discussion of chemical results calls for a study of the symmetry properties of graphs. In graphs we are concerned with the *connectivity*, and normally the angles and lengths of the links (edges) do not enter into consideration. Hence, one can view the pictorial diagrams of graphs as structures with even greater flexibility than non-rigid molecules. Symmetry properties of graphs will therefore be described by more versatile subgroups of the full permutational group. It is the purpose of this series of papers to discuss and describe the symmetry properties of graphs, in particular graphs of interest to chemistry. While in the case of nonrigid molecules it was possible to recognize additional symmetry operations, in contrast here with graphs, no previous knowledge of all feasible symmetry operations is available. Hence the study of the symmetry properties of graphs cannot follow the familiar procedure

* Dedicated to Professor Vladimir Prelog.

valid for molecules in which one examines which of the possible symmetry operations will leave the system invariant. The complexity of the symmetry properties of graphs is well illustrated in Figure 1 which depicts a graph of

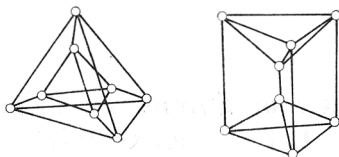


Figure 1. A similar graph shown as two interlocked tetrahedra and in a prismatic form

two interlocked tetrahedra (left side). Consider now as a new additional symmetry operation an inside-outside inversion by which the inner tetrahedron becomes outer and vice versa. By such an operation we have left the connectivity intact, hence it qualifies as a permissible symmetry operation. However, in addition to this operation we can pull the inside tetrahedron in such a way the two tetrahedra are not interlocked. In this way we obtain a prismatic structure (Figure 1, right side) in which also all connectivity is preserved. The new structure has a different geometric form and belongs to a different molecular point group. Hence, the considered graph has, simultaneously, symmetry properties of a tetrahedral structure and of a prismatic, and possibly a few others. Various pictorial representations of a graph only show some aspects of the underlying symmetry and the problem is to derive all the symmetry features of graphs of interest in a systematic way. We deal here with subgroups of the full symmetric group of all permutations, and since any subgroup of the full permutation group corresponds to a graph⁵ we may refer to the derived symmetry groups as the *connectivity groups*, in order to discriminate between these and other subgroups of the full symmetric group corresponding to *molecular point groups* and *non-rigid molecular symmetry groups*.

There are very few publications dealing with the symmetry properties of graphs in which the individual symmetry operations are fully indicated. Most of the mathematical papers, when applied to specific graphs, discuss only the order of the symmetry group, i. e., the number of the symmetry operations, and do not attempt to enlist the permutations involved. "Although not a profound task, the manual enumerations of the symmetries would be tedious and an algorithm approach would be preferred."⁶ While for smaller graphs the permutations of the labels that preserve the adjacency relationship may be apparent, this is no longer obvious in larger graphs and the necessity for a systematic approach becomes evident. For a number of smaller graphs Balaban⁷ tabulated the symmetry operations by listing the admissible permutations of labels. From such a list one can derive the cycle index term y_k which appears in Pólya's counting theorem⁸ and from which, as shown by Pólya, the number of substitutional isomers of the corresponding figure can be obtained. The cycle indices reflect *connectivity* rather than geometrical features, expressing constitutional isomerism. Lederberg⁶ considers somewhat larger graphs for which one can no longer operate solely on a visual image and describes an algorithm which exploits the hamiltonian circuit (where they exist). The essential feature

of the scheme is that it searches at most 2^n possibilities of label permutations rather than $n!$ possibilities which a complete exhaustion of label permutations involves.

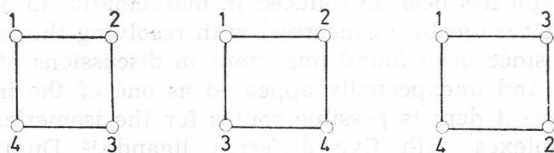
The strategy of our approach is different: rather than generating numerous (even if selective) permutations and subsequently testing to find which correspond to a symmetry operation of the graph, we derive acceptable labels, from which all symmetry operations follow.

OUTLINE OF THE PROCEDURE

It is known⁹ that finding all distinctive labelings of a graph which give a same adjacency matrix is tantamount to finding all the symmetry features of a graph. The individual symmetry operations correspond to the changes from one to another acceptable labeling. A list of all symmetry operations can be derived by indicating the permutations of labels between one of the labelings and all others. From such a list one can then construct the group multiplication table which may be viewed as the end of the task of characterizing the symmetry of a graph.

The problem consists in *finding* all labelings which belong to an identical adjacency matrix in a *practical* way. This excludes generating all $n!$ labelings and the subsequent search for those which have an identical adjacency matrix. A practical approach has to reduce the number of combinatorial possibilities that one examines dramatically. We will describe a scheme which satisfies the above requirement.

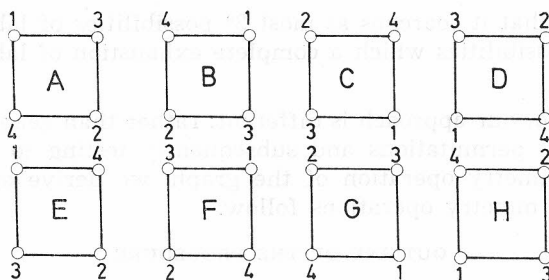
Let us illustrate the situation on a very simple graph of a square. There are in all $4! = 24$ distinctive labelings for the four vertices of a square, but as one can easily verify there are only three different adjacency matrices for the graph, since the position of the first label when all vertices are equivalent is immaterial (four possibilities) and the sense of direction along the cyclic system (clockwise or counterclockwise) will not affect the form of the matrix (two possibilities). Hence any of the shown three different labelings will generate another eight labelings which will not change the adjacency matrix:



The corresponding adjacency matrices are:

$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

Take for instance the last matrix and all the eight corresponding labelings:



By comparing the first labeling with itself and all others, the list of all the permutations of the labels which define the symmetry of the square are derived:

AA (1)(2)(3)(4)	AE (1)(2)(3, 4)
AB (4, 2, 3, 1)	AF (3, 1)(4, 2)
AC (2, 1)(4, 3)	AG (2, 1)(3)(4)
AD (3, 2, 4, 1)	AH (4, 1)(2, 3)

Any of the three adjacency matrices can be used for generating the permutations which would duplicate the results of others. For instance the permutations defining the symmetry of a square given by Balaban⁷ in his Table I correspond to the second adjacency matrix. Hence, if we consider only labelings that belong to one of the possible adjacency matrices all the duplications associated with the other forms of the adjacency matrix will be avoided resulting in an enormous saving of the searching for symmetry operations. As discussed elsewhere,¹⁰ it is possible to single out one of the different adjacency matrices because of its unique feature that it corresponds to the smallest binary code, if the rows of the matrix are combined in a single number, by sequencing them starting from the top, in a single line. Of the three matrices considered before, the last one, as one can easily verify, corresponds to the smallest binary code:

0 0 1 1 0 0 1 1 1 1 0 0 1 1 0 0

PETERSEN'S GRAPH

Petersen's graph has been introduced in mathematics to provide a counterexample to the Tait conjecture concerned with resolving the famous four color problem.¹¹ It has since been found important in discussions of various mathematical problems and unexpectedly appeared as one of the important graphs in chemistry where it depicts possible routes for the isomerization of trigonal bipyramidal complexes with five different ligands.¹² Dunitz and Prelog¹³ have pointed to the equivalence of various pictorial forms for the graph, in particular drawing attention to an alternative pentagonal form equivalent to the usually adopted trigonal representation for the graph in chemical literature. The equivalence between the pentagonal and trigonal forms has been known to mathematicians¹⁴, while the octahedral form for the graph does not appear in mathematical discussions.

The possibility of the plurality of pictorial forms for a similar connectivity which has different apparent symmetry is interesting, however there has been little systematic search for a characterization of the symmetry properties of

such graphs. In Figure 2 we illustrate the connectivity of the Petersen graph by different images having apparent symmetry D_{3h} , D_{5h} , T_d , and D_{2d} . Obviously the Petersen graph has all the symmetry properties following from the above representations, at which one may look as special subgroups of the actual symmetry group of the graph. Our task is to find the symmetry group in question and fully list all the permissible permutations of labels within the given symmetry group. For the Petersen graph it is known that the order of the symmetry group is 120 and that the group is fully symmetric (permutation) on five objects, S_5 . So in this particular application of our general approach to the characterization of the symmetry of graph novel results is the list of all symmetry operations.

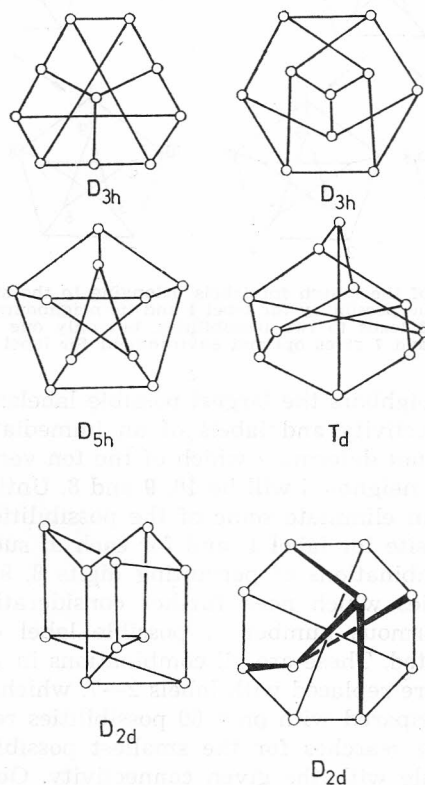


Figure 2. Geometrical representations of the Petersen graph of different apparent symmetry

First, we have to find the canonical numberings of the vertices associated with the smallest binary code for the adjacency matrix when its entries are read row by row from left to right and from top to bottom. In Figure 3 we illustrate the search for the canonical labeling. In order that the code is as small as possible obviously *the first row* of the adjacency matrix should have as many zeros as possible and these should all precede the digits of one. Such a distribution of labels will secure that the beginning of the overall label ensures the possible smallest binary code. Hence the smallest label 1 should

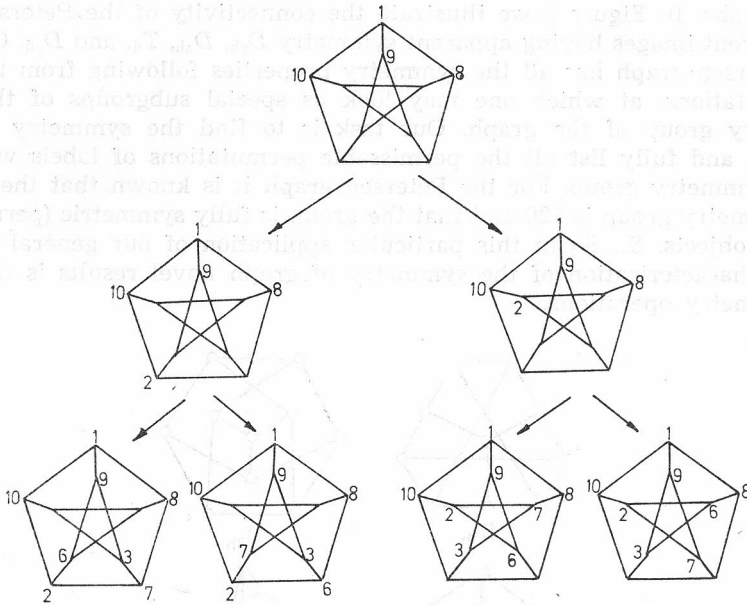


Figure 3. An illustration of the search for labels belonging to the smallest binary code for the adjacency matrix. Only one possibility for label 1 and its neighbours 10, 9, 8 is shown (out of 60 such possibilities). Label 2 leads to two possibilities, but only one alternative assignment of 6 and 7 gives optimal environment for label 3.

have as its nearest neighbors the largest possible labels: 10, 9, 8. The condition determines the connectivity and labels of an immediate environment of the vertex 1, but it does not determine which of the ten vertices should be labeled as 1 and which of its neighbors will be 10, 9 and 8. Until from some additional considerations one can eliminate some of the possibilities, one has to consider all ten vertices as a site for label 1, and for each of such possibilities one has to register all $3!$ combinations of permuting digits 8, 9, 10. Despite the large number of possibilities which need further consideration one should realize that already an enormous number of possible label distributions, which is $10!$, has been eliminated. These are all combinations in which any or all of the large labels 8, 9, 10 are replaced with labels 2—7, which gives more than 30000 possibilities to be compared with only 60 possibilities retained in the analysis. In the next step one searches for the smallest possible binary code for the second row compatible with the given connectivity. Obviously label 2 should be adjacent to label 10 since only then the second row will produce the smallest number. Its neighbors will have the largest available labels which are now 6 and 7. A closer examination of Figure 3, which depicts one of the acceptable labelings for 1 and the triplet 10, 9, 8, now reveals that label 2 has two possible sites. An assignment of label 2 to any of the two sites gives two possibilities for the assignment of labels 6 and 7. However, as one can verify quickly only one of the two possibilities for placing labels 6 and 7 leads to the smallest value for the third row of the adjacency matrix. The situation is shown in Figure 3, where one see that the two alternative assignments of labels 6 and 7 produce a *different* environment for label 3. In one case 3 has as neighbors

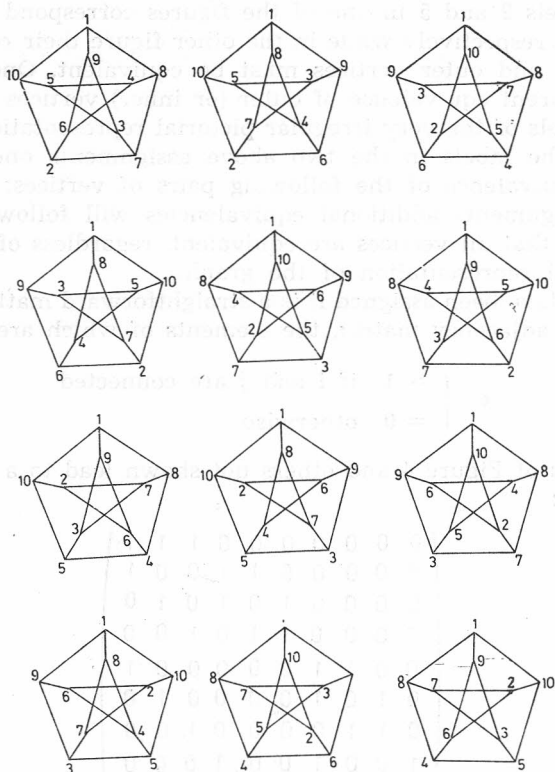
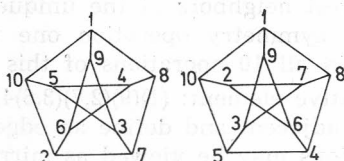


Figure 4. Twelve labelings of vertices of the Petersen graph derived from a fixed site for label 1. The remaining of 120 labelings follow from a different selection of the site for label 1.

5, 7, 9 while in the other case its neighbors are 5, 6, 9, clearly the former corresponds to the smaller value for the third row. In the continuation of the search for the canonical labels unacceptable assignments are abandoned and one continues with the assignment of yet unused labels. For this particular example all subsequent labels have a unique position already determined with the assignment of labels 1, 10, 9, 8, and 2. In Figure 4 we list twelve out of possible 120 labelings which are given by selecting a site for label 1. Other possibilities can be derived from those given in Figure 4 by selecting any of the remaining nine vertices as the site for label 1. Observe that in deriving acceptable labelings no use of the apparent symmetry of Petersen's graph was made. However, from derived labeling, one can deduce immediately that all vertices in this highly symmetrical graph are equivalent. Take for example the two acceptable labelings of Figure 4:



We see that labels 2 and 5 in one of the figures correspond to an outer and the inner vertex respectively while in the other figure their role is exchanged, hence the inner and outer vertices must be equivalent. One even need not assume the apparent equivalence of outer (or inner) vertices and their use in deriving the labels of the very irregular pictorial representations of the graph. By comparing the labels in the two above assignments one can univocally establish the equivalence of the following pairs of vertices: (2,5); (3,6); (4,7). From other assignments additional equivalencies will follow and eventually one will deduce that all vertices are equivalent, regardless of the form of the adopted pictorial representation of the graph.

Once labels have been assigned it is a straightforward matter to write down the form of the adjacency matrix, the elements of which are defined by:

$$a_{ij} \begin{cases} = 1 & \text{if } i \text{ and } j \text{ are connected} \\ = 0 & \text{otherwise} \end{cases}$$

All the labelings of Figure 4 and others not shown lead to a single adjacency matrix which is:

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

LIST OF SYMMETRY OPERATIONS

The list of symmetry operations can be constructed once we have all labelings belonging to the same adjacency matrix. All 120 symmetry operations fall into seven classes of the symmetry group. Each class is characterized by a partitioning of the permutations in cycles, giving:

$$1^{10} \quad 1^4 2^3 \quad 1^2 2^4 \quad 1 3^3 \quad 1 3 6 \quad 2 4^2 \quad 5^2$$

The number of symmetry operations within each class can be determined from a closer look at the permutations involved (Figure 4):

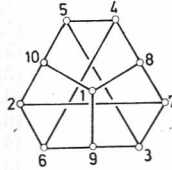
1^{10} this is identity operation, each label is unpermuted;

$1^4 2^3$ take as representative element: (1)(8)(9)(10)(2,5)(3,6)(4,7) Vertex (1) has here a unique position, its nearest neighbors also remain unpermuted, while the next nearest neighbors of the unique vertex exchange labels. Since in each such symmetry operation one vertex takes the unique position, there are in all 10 operations of this class;

$1^2 2^4$ take as a representative element: (1)(9)(2,7)(3,6)(4,5)(8,10). The unpermuted pair of vertices are adjacent and define an edge. The remaining vertices that exchange positions may be viewed as mirror images in a reflection

plane which contains the unique edge. Since there are 15 edges in the graph, each will take the unique position in one of the operations of the class, hence there are 15 operations in this class;

1 3³ take as representative element: (1)(2,4,3)(5,7,6)(8,9,10). One vertex takes the unique position (being unpermuted), the remaining are cyclically permuted, suggesting the rotation of a figure about a threefold axis. Visualization of such operations is therefore simple if the graph is represented by a figure with a threefold axis:



There are ten vertices, but two senses of rotation, which leads to 20 symmetry elements in this class;

1 3 6 take as a representative element: (1)(8,9,10)(2,7,3,5,4,6). Again there is a single unique vertex and a cyclic permutation of three labels adjacent to the unique site (with the remaining vertices making another cyclic permutation) which can be associated with a positive and negative sense of rotation. Hence, again there will be 20 symmetry elements in this class also;

2 4² take as a representative element: (1,9)(2,4,7,5)(3,10,6,8). Here an edge plays the unique role, while other vertices fall in group of four which are cyclically permuted. There are two senses of cyclic permutations and in all 15 edges which makes a total of 30 symmetry operations in this class. One can visualize the individual permutations best in a figure of D_{2d} apparent symmetry;

TABLE I

List of all 120 Symmetry Operations of the Petersen Graph. Operations Belonging to the same Class are Grouped together.

Permutations	
1^{10}	$1^2 2^4$
(1)(2)(3)(4)(5)(6)(7)(8)(9)(10)	(1)(8)(2,6)(3,5)(4,7)(9,10) (1)(10)(2,5)(3,7)(4,6)(8,9) (2)(7)(1,9)(4,5)(6,10)(3,8) (1)(9)(2,7)(3,6)(4,5)(8,10) (4)(5)(1,9)(2,7)(3,10)(6,8) (2)(10)(1,5)(3,9)(4,8)(6,7) (2)(6)(1,8)(3,5)(4,9)(7,10) (3)(5)(1,8)(2,6)(4,10)(7,9) (7)(8)(1,4)(2,3)(5,10)(6,9) (3)(7)(1,10)(2,8)(4,6)(5,9) (4)(6)(1,10)(2,9)(3,7)(5,8) (4)(8)(1,7)(2,10)(3,9)(5,6) (6)(8)(1,3)(2,4)(5,10)(7,8) (5)(10)(1,2)(3,4)(6,9)(7,8) (3)(9)(1,6)(2,10)(4,8)(5,7)
$1^4 2^3$	
(1)(2)(5)(10)(3,4)(6,7)(8,9) (1)(8)(9)(10)(2,5)(3,6)(4,7) (1)(4)(7)(8)(2,3)(5,6)(9,10) (1)(3)(6)(9)(2,4)(5,7)(8,10) (2)(3)(7)(8)(1,4)(5,9)(6,10) (2)(6)(7)(10)(1,5)(3,8)(4,9) (3)(5)(7)(9)(1,6)(2,8)(4,10) (4)(5)(6)(8)(1,7)(2,9)(3,10) (2)(4)(6)(9)(1,3)(5,8)(7,10) (3)(4)(5)(10)(1,2)(6,8)(7,9)	

Table I, contd.

	$1 \quad 3^3$	
(1)(2,4,3)(5,7,6)(8,9,10)		(4,8)(1,6,7,5)(2,3,10,9)
(1)(2,3,4)(5,6,7)(8,10,9)		(2,7)(1,4,9,5)(3,10,8,6)
(6)(1,7,5)(2,4,9)(3,10,8)		(1,8)(2,5,6,3)(4,9,7,10)
(8)(1,7,4)(2,5,9)(3,6,10)		(1,8)(2,3,6,5)(4,10,7,9)
(3)(1,2,4)(5,9,7)(6,8,10)		(3,7)(1,6,10,4)(2,5,8,9)
(7)(1,6,5)(2,3,8)(4,10,9)		(6,9)(1,2,3,4)(5,8,10,7)
(10)(1,2,5)(3,8,6)(4,9,7)		(5,10)(1,3,2,4)(6,8,9,7)
(3)(1,4,2)(5,7,9)(6,10,8)		(2,7)(1,5,9,4)(3,6,8,10)
(4)(1,3,2)(5,6,8)(7,10,9)		(1,10)(2,9,5,8)(3,4,7,6)
(9)(1,3,6)(2,8,5)(4,10,7)		(1,10)(2,8,5,9)(3,6,7,4)
(5)(1,7,6)(2,9,8)(3,4,10)		(2,6)(1,3,8,5)(4,10,8,7)
(8)(1,4,7)(2,9,5)(3,10,6)		(3,9)(1,7,6,5)(2,4,10,8)
(2)(1,4,3)(5,9,8)(6,7,10)		(3,5)(1,6,8,2)(4,7,10,9)
(5)(1,6,7)(2,8,9)(3,10,4)		(6,9)(1,4,3,2)(5,7,10,8)
(6)(1,5,7)(2,9,4)(3,8,10)		(4,5)(1,7,9,2)(3,6,10,8)
(4)(1,2,3)(5,8,6)(7,9,10)		(3,7)(1,4,10,6)(2,9,8,5)
(9)(1,6,3)(2,5,8)(4,7,10)		(2,10)(1,7,5,6)(3,4,9,8)
(10)(1,5,2)(3,6,8)(4,7,9)		(2,10)(1,6,5,7)(3,8,9,4)
(7)(1,5,6)(2,8,3)(4,9,10)		(5,10)(1,4,2,3)(6,7,9,8)
(2)(1,3,4)(5,8,9)(6,10,7)		(4,6)(1,7,10,3)(2,5,9,8)
		(4,5)(1,2,9,7)(3,8,10,6)
		(3,9)(1,5,6,7)(2,8,10,4)
		(4,6)(1,3,10,7)(2,8,9,5)
		(2,6)(1,5,8,3)(4,7,9,10)
		(7,8)(1,2,4,3)(5,9,10,6)
		(7,8)(1,3,4,2)(5,6,10,9)
		(4,8)(1,5,7,6)(2,9,10,3)
	$1 \quad 3 \quad 6$	
(7)(2,3,8)(1,10,5,4,6,9)		
(2)(6,10,7)(1,8,4,5,3,9)		
(1)(8,10,9)(2,6,4,5,3,7)		
(1)(8,9,10)(2,7,3,5,4,6)		
(4)(5,6,8)(1,10,2,7,3,9)		
(5)(3,10,4)(1,8,7,2,6,9)		
(4)(5,8,6)(1,9,3,7,2,10)		
(3)(5,9,7)(1,8,4,6,2,10)		
(6)(2,9,4)(1,8,7,3,5,10)		
(10)(1,2,5)(3,9,6,4,8,7)		
(2)(6,7,10)(1,9,3,5,4,8)		
(3)(5,7,9)(1,10,2,6,4,8)		
(6)(2,4,9)(1,10,5,3,7,8)		
(5)(3,4,10)(1,9,6,2,7,8)		
(8)(1,7,4)(2,6,9,3,5,10)		
(7)(2,8,3)(1,9,6,4,5,10)		
(8)(1,4,7)(2,10,5,3,9,6)		
(9)(1,6,3)(2,7,8,4,5,10)		
(10)(1,5,2)(3,7,8,4,6,9)		
(9)(1,3,6)(2,10,5,4,8,7)		
		5^2
		(1,8,7,3,9)(2,5,6,10,4)
		(1,10,2,6,9)(3,8,5,7,4)
		(1,8,4,6,9)(2,3,10,7,5)
		(1,10,5,3,9)(2,4,7,6,8)
		(1,8,7,2,10)(3,6,5,9,4)
		(1,8,4,5,10)(2,9,7,6,3)
		(1,9,6,2,10)(3,4,7,5,8)
		(1,3,10,9,5)(2,6,4,8,7)
		(1,9,6,4,8)(2,5,7,10,3)
		(1,5,8,10,4)(2,6,9,3,7)
		(1,10,2,7,8)(3,4,9,5,6)
		(1,9,3,7,8)(2,4,10,6,5)
		(1,10,5,4,8)(2,3,6,7,9)
		(1,6,8,9,4)(2,7,3,5,10)
		(1,9,3,5,10)(2,8,6,7,4)
		(1,4,10,8,5)(2,7,3,9,6)
		(1,7,10,8,2)(3,5,4,6,9)
		(1,4,9,8,6)(2,10,5,3,7)
		(1,3,8,9,7)(2,10,5,4,6)
		(1,7,9,8,3)(2,6,4,5,10)
		(1,2,8,10,7)(3,9,6,4,5)
		(1,5,9,10,3)(2,7,8,4,6)
(3,5)(1,2,8,6)(4,9,10,7)		(1,6,10,9,2)(3,7,8,4,5)
(1,9)(2,5,7,4)(3,8,6,10)		(1,2,9,10,6)(3,5,4,8,7)
(1,9)(2,4,7,5)(3,10,6,8)		
	$2 \quad 4^2$	
(3,5)(1,2,8,6)(4,9,10,7)		
(1,9)(2,5,7,4)(3,8,6,10)		
(1,9)(2,4,7,5)(3,10,6,8)		

²⁵ take as a representative element: (1,10,2,7,8)(3,4,9,5,6). The presence of five vertices in a cyclic permutation suggests the visualization of the symmetry operations figure with a pronounced fivefold rotational axis. There are 12 five membered rings¹⁵ in the graph which can be posed in the unique position and for each, one can have rotation in the positive or the negative sense for an angle of $2\pi/5$. In all this makes 24 symmetry elements in this class. Observe that the remaining five vertices which also cyclically change labels are not adjacent to each other. This makes a rotation by 2 ($2\pi/5$) to correspond to the rotation of the other set of five vertices by $2\pi/5$, hence there is no need to consider the successive rotations about the fivefold axis.

As we see, all the symmetry operations can be interpreted with known operations of symmetry points group if a suitable geometrical realization of the graph is selected.

DISCUSSION

Symmetry of the Petersen graph has been investigated by mathematicians and that it is a full symmetric group S_5 is known.¹⁶ The equivalence with the S_5 group can be easily established if one considers the particular contractions of the graph in which the length of selected edges is gradually reduced until the corresponding adjacent vertice collapses into a single vertex.¹⁷ Consider the graph with the pentagonal image and gradually reduce the lengths of the radial edges connecting the inner folded ring with the outer five membered ring. As a result we have a complete graph with five vertices K_5 , which of course belong to the full symmetry group S_5 . Each labeled Petersen graph will, through such a process, be transformed into a labeled complete graph in which each vertex will have double labels. If one retains only the smaller label, then for selected cases we obtain the labeled graphs of Figure 5. The process illustrates that there is a 1 : 1 correspondence between the two sets of labeled graphs.

Previous work on the symmetry properties of the Petersen graph was directed to establish its isomorphism with the group of the complete graph K_5 which then has $5! = 120$ symmetry operations. We presented here the list of all operations. Classes in the full symmetric group are determined by the partition of the permutations, but this need no longer hold in subgroups of the full symmetric group which may correspond to the symmetry of other graphs. Our approach is sufficiently general to yield results also for graphs which have a lesser symmetry than complete graphs. The symmetry operations of the Petersen graph can be interpreted within forms for the graph which have an apparent symmetry D_{5h} , D_{3d} , or D_{2d} . Since D_{3d} and D_{2d} are subgroups of the tetrahedral point group T_d we may summarize the symmetry properties of the Petersen graph by indicating that within itself it contains point symmetry groups T_d and D_{5h} . For the connectivity group of the Petersen graph we may symbolically write (T_d, D_{5h}) . The two point groups only indicate the fragmentary symmetry features of the Petersen graph, but the notation has a convenient property: it indicated the highest symmetries of the geometrical figures that one can construct to represent the graph and its connectivity. Any isomorphous group to those shown will lead to alternative geometrical forms, while any subgroup of the point groups listed in the bracket will suggest geometrical forms of *lower* apparent symmetry. Thus since D_{3d} is a subgroup of T_d one

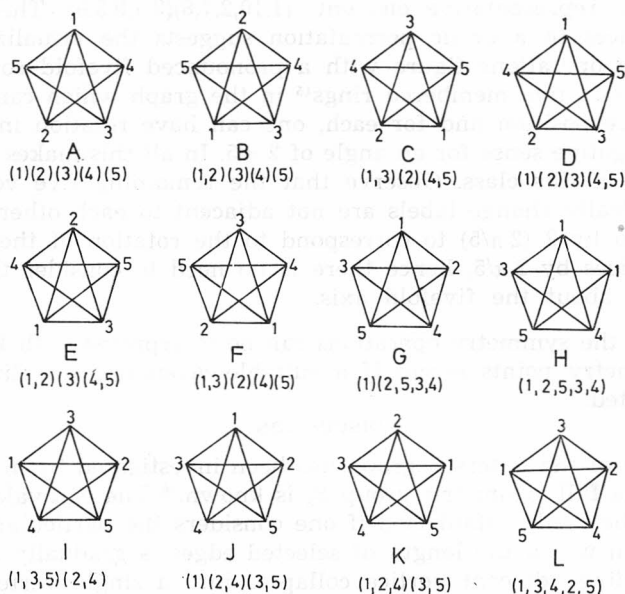


Figure 5. Contracted graphs derived from the fusion of five pairs of adjacent vertices which convert the Petersen graph into the complete graph on five vertices (K_5). There is a 1:1 correspondence between each labeled Petersen graph and the corresponding labeled K_5 graph.

can construct a figure D_{3d} symmetry if one wishes. Since D_{3d} is isomorphic with D_{3h} one can make a geometrical figure of the Petersen graph of apparent D_{3h} symmetry. Such forms have been frequently used in chemical literature, in particular before the symmetry properties of the Petersen graph were better investigated.

Acknowledgment. I would like to thank professor A. T. Balaban (Bucharest, Roumania) for discussion of the material and several suggestions that improved the presentation. Also I am indebted to professor J. Lederberg (Stanford Univ.) for kindly sending preprints concerning use of graphs in the analysis of the ring structures of chemistry, (ref. 6 in particular). This work was supported by the U.S. Department of Energy, Division of Basic Energy Sciences.

REFERENCES

1. J. B. Howard, *J. Chem. Phys.*
2. E. B. Wilson Jr., C. C. Lin, and D. R. Lide, *J. Chem. Phys.* **23**, 136 (1955).
3. J. T. Hougen, *J. Chem. Phys.* **37** (1962) 1433; **39** (1963) 358.
4. H. C. Longuet-Higgins, *Mol. Phys.* **6** (1963) 445.
5. R. Frucht, *Compositio Math.* **6** (1938) 239.
6. J. Lederberg, *Dendral-64, Part II* a report to National Aeronautics and Space Administration, NASA CR 68898.
7. A. T. Balaban, *Rev. Roum. Chim.* **19** (1974) 1323.
8. G. Pólya, *Acta Math.* **68** (1937) 145.
9. F. Harary, *Graph Theory*, Addison-Wesley Publ. Co., Reading, Mass, 1972, chapter 14.
10. M. Randić, *J. Chem. Inf. & Computer Sci.* **17** (1977) 171.
11. See: N. L. Biggs, E. K. Lloyd, and R. J. Wilson, *Graph Theory* **1736—1936**, Clarendon Press, Oxford 1976.

12. M. Gielen and J. Nasielski, *Bull. Soc. Chim. Belges* **78** (1969) 339; J. Brocas and M. Gielen, *Bull. Soc. Chim. Belges* **80** (1971) 207.
13. J. D. Dunitz and V. Prelog, *Angew. Chem.* **80** (1968) 700.
14. W. T. Tutte, *Connectivity in Graphs*, Univ. of Toronto Press, Toronto 1966.
15. There are 10 vertices, each vertex is involved in 6 five membered rings, which total 60. However each ring has been counted five times (having five vertices) once for each vertex of the ring, hence the result is $60/5$, i. e., 12.
16. R. Frucht, *Comment. Math. Helv.* **9** (1937) 217.
17. F. Harary and W. T. Tutte, *Canad. Math. Bull.* **8** (1965) 17.

SAŽETAK

Sustavni studij simetrijskih svojstava grafova. I. Petersonov graf

M. Randić

Izvedena su simetrijska svojstva Petersonova grafa s pomoću jednostavnog postupka. Taj se postupak temelji na traženju svih numeriranja grafa, koji imaju jedinstvenu matricu susjedstva. Petersonov graf je važan pri proučavanju izomerizacija trigonalnih bipiramidskih kompleksa s pet različitih liganada.

AMES LABORATORY-USDOE, IOWA STATE
UNIVERSITY, AMES, IOWA 50011, U.S.A.

Prispjelo 12. prosinca 1976.