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Chemical applications of topology and group theory

19. The even permutations of the ligands in five-coordinate complexes viewed as proper rotations of the regular icosahedron [1]

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The 60 even permutations of the ligands in the five-coordinate complexes, ML_5, form the alternating group A_5, which is isomorphic with the icosahedral pure rotation group I. Using this idea, it is shown how a regular icosahedron can be used as a topological representation for isomerizations of the five-coordinate complexes, ML_5, involving only even permutations if the five ligands L correspond either to the five nested octahedra with vertices located at the midpoints of the 30 edges of the icosahedron or to the five regular tetrahedra with vertices located at the midpoints of the 20 faces of the icosahedron. However, the 120 total permutations of the ligands in five-coordinate complexes ML_5 cannot be analogously represented by operations in the full icosahedral point group I_h, since I_h is the direct product $I \times C_2$ whereas the symmetric group S_5 is only the semi-direct product $A_5 \wedge S_2$. In connection with previously used topological representations on isomerism in five-coordinate complexes, it is noted that the automorphism groups of the Petersen graph and the Desargues–Levi graph are isomorphic to the symmetric group S_5 and to the direct product $S_5 \times S_2$, respectively. Applications to various fields of chemistry are briefly outlined.

Key words: Pentacoordinate complexes — Ligand permutation — Group theory — Graph theory — Isomerization processes

Introduction

The marked resurgence of interest in chemical graph theory [2, 3] over the past decade has brought in its wake an ever increasing number of new applications, ranging from isomer enumerations [4], through bonding theory applications [5, 6] and the investigation of reaction networks [7–9], to the characterization of chemical species by topological indices [10]. One application of importance which has recently come to the fore [11, 12] concerns the use of graphs to represent the various transformations, such as interconversions or isomerizations, which non-rigid chemical species can undergo. Graphs of this type have been referred to as *topological representations* [13]. This line of research was first initiated by Balaban and co-workers [14], who used isomerization graphs to represent the 1,2-charge migrations occurring in $CH_3CH_2^+$ carbonium ions. The graph they employed for this purpose is known as the Desargues–Levi graph, a graph which has since been shown to have several other applications in chemistry, such as the representation of the rearrangements of the ML_5 trigonal bipyramidal complexes [15, 16]. It was soon demonstrated that a closely related graph, the Petersen graph, can be used for the same purpose if no discrimination of the enantiomers is required. Randić has investigated both the Desargues–Levi [17] and Petersen [18] graphs, especially in regard to their role in elucidating complex chemical relations.

The visualization of chemical transformations which graphs make possible has led fairly naturally to the use of graph vertices for the purpose of representing isomers which arise from the possible permutations of species or ligands. By the same token, graph edges have been associated with the isomerization processes taking place. Hence, the various applications of chemical graphs in this area require knowledge of the symmetry properties of graphs. Clearly, an appropriate use of group theory to study the symmetry properties of such graphs will enable deductions to be made concerning the symmetry of the transformations involved. Now, it is well-known that the symmetry elements of a graph do not depend on the manner in which the graph is depicted but rather on its neighborhood relationships, i.e. the connectivity or, more loosely, the topology, it expresses. Thus, although the same graph may be drawn in several different ways, each of which shows an apparently different symmetry, its actual symmetry will in fact depend on which vertices of the graph are connected together and which are not. As an illustration of this point, we present in Fig. 1 three differing representations of the Desargues–Levi graph displaying three apparently different symmetries.

The representation adopted in practice for a given chemical graph will depend primarily on its value in illustrating the specific chemical problem under investigation. Balaban [19], however, has proposed that the criteria adopted be based on both scientific and aesthetic considerations. An appropriate type of representation should take the cognizance of the following prescriptive criteria:

1) display the graph, if possible, with a Hamiltonian circuit;
2) exploit the particular chemical interpretation to the full;
3) exhibit as high a degree of symmetry as possible.

Frequently, it is not possible to satisfy all three of these criteria simultaneously, either as a result of mutual conflicts in these requirements or because of the absence of some symmetry elements in the graphs themselves. In practice, however, it is possible in most cases to satisfy at least two of them.

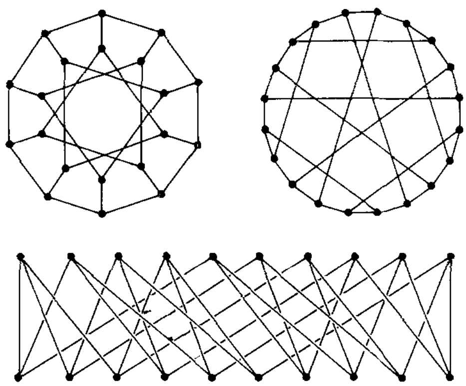

Fig. 1. Three different pictures of the Desargues–Levi graph showing three apparently differing symmetries

In the graphs discussed in this paper, it is possible to satisfy all three of the above criteria. We shall be examining relationships existing between the permutations of the five ligands in ML_5 complexes and the proper rotations of the regular icosahedron. The relevant graphs involved here are the Desargues-Levi graph (or, alternatively, the Petersen graph) and that of the icosahedron. All three of these graphs display a high degree of symmetry. Moreover, the Desargues-Levi and icosahedral graphs are possessed of a Hamiltonian circuit, although the Petersen graph contains no such circuit. The Desargues-Levi graph has a total of 240 symmetry operations partitioned into 14 classes; the Petersen graph belongs to a symmetry group of 120 and is partitioned into 7 classes [11]. The chemical significance of all three graphs is now well-established and is exploited in the present study.

The role of simplexes

A number of workers [20-23] have related the permutation groups on sets of identical ligands to the symmetry point groups on the various ML_n species. Special interest has focused on the species with $5 \leq n \leq 6$ for two principal reasons. First, these complexes have been studied very extensively by experimental chemists; and second, when $n < 5$ there is little need to introduce graphs to represent the possible geometric isomers in view of the extreme simplicity of the systems involved. If we consider complexes with $3 \leq n \leq 6$ exhibiting skeletons of the highest possible symmetry, the triangular ML_3 complex will be of D_{3h} symmetry and have only one isomeric form even if the three ligands L are nonequivalent. The tetrahedral form adopted by ML_4 complexes, which is of T_d symmetry, can give rise to only two geometric isomers, corresponding to the two enantiomers of an asymmetric carbon atom, even if all four of the ligands L are nonequivalent. When we reach the trigonal bipyramid ML_5 of D_{3h} symmetry, the number of possible geometric isomers increases to 20 in the case where all the five ligands are nonequivalent [4]. Similarly, for octahedral ML_6 complexes of O_h symmetry the number of geometric isomers equals 30 when all six ligands are nonequivalent. Thus five and six are the minimum coordination numbers, n, in the most symmetrical ML_n complexes for which the graphs representing their rearrangements become nontrivial.

The alternating group A_3 and the symmetric group S_3 on three objects are isomorphic with the point groups C_3 and D_3, respectively. The latter two point groups correspond to the symmetry of the two-dimensional simplex [24], i.e. to the planar triangle found in ML_3 derivatives such as the boron trihalides. Similarly, the alternating group A_4 and the symmetric group S_4 are, respectively, isomorphic with the point groups T and T_d, which correspond to the symmetry of the three-dimensional simplex, i.e. to that of the regular tetrahedron found in many ML_4 derivatives as well as to the sp^3 carbon atoms in organic derivatives. By direct analogy with the permutation groups on three and four objects, we would expect the A_5 and S_5 permutation groups to display isomorphism with the symmetry of the four-dimensional simplex, of which the non-planar complete graph K_5 [25] is the 1-skeleton [24]. Yet, although this expectation is in fact fulfilled, it turns out to be neither very useful nor particularly relevant in the present context.

The practical implications

Accordingly, we shall discuss here the problem of how to treat the isomorphism of the alternating group A_5 and the symmetric group S_5 on five objects with various symmetry point groups in a chemically meaningful way. Of considerable interest is the relationship existing between the permutation groups A_5 and S_5 and the point group symmetries of actual three-dimensional figures. Now, the only conceivable three-dimensional point groups which could be related to the A_5 and S_5 permutation groups are, respectively, the I and I_h point groups. These represent the symmetry of the regular icosahedron and that of its dual graph [24], the pentagonal dodecahedron, respectively. The regular icosahedron has 12 vertices, 30 edges, and 20 faces; the pentagonal dodecahedron has 20 vertices, 30 edges, and 12 faces.

An analysis of the kind presented here can provide valuable new insights into a number of problems of considerable current interest. In our introduction we have already mentioned the use of graphs for the visualization of chemical transformations. This approach has been adopted by Balaban [19], Muetterties [20], and Gielen and Depasse-Delit [21], among others, for the depiction of intramolecular isomerizations of octahedral complexes which occur via twisting mechanisms. The symmetry of such graphs has aided greatly in achieving self-consistent notations for the various isomeric species involved. Moreover, in the field of crystallography [26-29], crystallographic orbits - also sometimes referred to as regular point systems or point configurations - and site symmetry groups are proving to be highly topical at present. So called "forbidden" fivefold symmetry has recently been observed in quasicrystals [30], a highly organized state of matter which is quite distinct from that in regular crystals or glasses. Structures possessing the rotational symmetry of the regular icosahedron, although forbidden in classical crystallography, have been discovered [31] in rapidly cooled melts of aluminum with an admixture of transition metals such as iron or manganese. Our analysis is also applicable to the study of electron and cage compounds. For instance, the larger sodium clusters, Na_{13} and Na_{13}^{+}, are known to possess icosahedral symmetry, whereas the smaller clusters, Na_7 and Na_7^{+}, have a pentagonal-pyramidal structure [32]. Other alkali clusters, e.g. the lithium clusters [33], appear to follow the same general pattern. Symmetry constraints are known to play a vital role in determining the equilibrium geometries of such species.

In the field of molecular biology, too, our analysis may have important implications. Crick and Watson [34] have convincingly argued that in biological systems such as viruses the protein molecules are likely to be positioned according to some underlying geometrical ground plan. High resolution cluster microscopy studies on isolated viruses have revealed that this is indeed the case for these systems. So-called "spherical" viruses are in fact based on one of three main geometrical plans and exhibit either helical, icosahedral, or complex symmetry. The basic model for a capsid having icosahedral symmetry has 12 morphological units in the form of pentamers located on the 12 fivefold rotational symmetry axes of an icosahedron. Systems of this particular type have been observed in the electron microscope [35], one such system being the comparatively well-known bacteriophage $\phi X174$. To determine the numbers of morphological units or capsomers for a given virus particle, it is necessary that at least two of the 12 fivefold rotational symmetry axes be identified. Analyses of the type we now present below could be very helpful in establishing this type of information.

Some applicable group theory

We now apply some basic group theory to the problem we have outlined above. Both the alternating group, A_5, and the pure rotation group, I, have a total of 60 symmetry operations. Similarly, both the symmetric group, S_5, and the full icosahedral point group, I_h, have 120 operations. Examination of the conjugacy class structure [26, 27] of the permutation groups A_5 and S_5 on the one hand, and that of the point groups I and I_h on the other hand, reveals that they correspond to each other. In fact, it is an elementary exercise to show [28] that:

$$I \cong A_5 \text{ (isomorphism)} \quad (1)$$

$$S_5 = A_5 \wedge S_2 \text{ (semi-direct product)} \quad (2)$$

$$I_h = I \times C_2 \text{ (direct product).} \quad (3)$$

In this context, a group G is a direct product of two groups A and B (i.e., $G = A \times B$) when:

1) for any $a \in A$ and any $b \in B$ the automorphism $\phi(b)$ of A is the identity thus:

$$\phi(b)a = a; \quad (4)$$

2) there is an isomorphism between G and the group of pairs (a, b), with $a \in A$ and $b \in B$, which satisfies the multiplication law:

$$(a_1, b_1)(a_2, b_2) = (a_1 a_2, b_1 b_2). \quad (5)$$

Similarly a group G is a semi-direct product of two groups A and B (i.e. $G = A \wedge B$) when:
1) for any $a \in A$ and any $b \in B$ there is an automorphism $\phi(b)$ of A such that:

$$\phi(b_1)[\phi(b_2)a] = \phi(b_1 b_2)a; \tag{6}$$

2) there is an isomorphism between G and the group of pairs (a, b) with $a \in A$ and $b \in B$ which satisfies the multiplication law:

$$(a_1, b_1)(a_2, b_2) = (a_1[\phi(b_1)a_2], b_1 b_2). \tag{7}$$

An automorphism of any group is an isomorphism with the graph itself. Two different numberings of the vertices which preserve the adjacency relationship will be an automorphism.

One of the present authors has recently discussed the concepts of direct products and semi-direct products of symmetry groups in another context [36].

Let us now consider the S_n permutation groups. In these groups permutations having different cycle structures will necessarily belong to different classes. Moreover, for these specific groups, a common partition will be a guarantee that the elements do in fact belong to the same class. Thus, the conjugacy classes of the permutation groups A_5 and S_5 are indicated in terms of their cycle indices [37, 38] in the following way:

$$60Z(A_5) = x_1^5 + 20x_1^2x_3 + 15x_1x_2^2 + 24x_5 \tag{8}$$

$$120Z(S_5) = x_1^5 + 10x_1^3x_2 + 20x_1^2x_3 + 15x_1x_2^2 + 30x_1x_4 + 20x_2x_3 + 24x_5. \tag{9}$$

Furthermore, the conjugacy classes [26, 27] of the point groups I and I_h are indicated from their character tables [39] to be the following:

$$I = \{E, 12C_5, 12C_5^2, 20C_3, 15C_2\} \tag{10}$$

$$I_h = \{E, 12C_5, 12C_5^2, 20C_3, i, 12S_{10}^3, 12S_{10}, 20S_6, 15\sigma\} \tag{11}$$

To avoid any confusion here, note that in Eq. (11), S_{10} and S_6 refer to improper rotations (rotation-reflections) rather than to symmetric groups.

It is now possible to compare Eqs. (8) and (9) with Eqs. (10) and (11), respectively, by using the relationships expressed in Eqs. (1), (2), and (3). This process of comparison leads to the following results:

1) the class of A_5 represented by the cycle index term $24x_5$ corresponds to the two classes $12C_5$ and $12C_5^2$ of I taken together;
2) in the point group I_h, each class of improper rotations (i, S_{10}, S_{10}^3, S_6 and σ) corresponds to a class of proper rotations of the same size, namely to (E, C_5, C_5^2, C_3, and C_2, respectively), whereas the classes of S_5 are not partitioned analogously.

Visualization of the operations

In order to delve further into and to facilitate visualization of the relationship between the alternating group A_5 and the icosahedral rotation subgroup I, the following approach is proposed. First, imagine five equivalent objects located on a body having I point group symmetry, such as a regular icosahedron or its dual [24], the regular pentagonal dodecahedron. The permutations which these five equivalent objects undergo as each of the rotations of I is applied to the body are then observed. This procedure should lead us directly to the desired relationship between the terms in the cycle index of A_5 and the rotations of I. By making use of the graph of the regular icosahedron, a method has been devised for the representation of the even permutations of five objects, indicated by the permutation group A_5, as the proper rotations of the regular icosahedron.

The construction of five equivalent objects from an icosahedron requires the utilization of five equivalent sets of either four faces or six edges. However, five equivalent objects cannot be constructed from the vertices of an icosahedron for the simple reason that 12 is not divisible by 5. The now classical work by Klein [40] on the icosahedron suggests the following prescription for partitioning the 30 edges of an icosahedron into five sets of six edges each:
1) draw a straight line from the midpoint of each edge through the center of the icosahedron to the midpoint of the unique opposite edge;
2) divide the resulting 15 straight lines into five sets of three mutually perpendicular straight lines. Then each set of three mutually perpendicular straight lines resembles a set of Cartesian coordinates and defines a regular octahedron.

Each of these octahedra can also be defined in terms of 12 faces of the underlying icosahedron, where the 12 faces are the six pairs meeting at the six edges, whose midpoints define the vertices of the octahedron as described above. Thus, in defining the complete icosahedral set of five octahedra in terms of the icosahedral faces, each face will be used $5 \times 12/20 = 3$ times.

The construction outlined above is actually the dual [24] of a construction described by DuVal [41] in which a regular dodecahedron is partitioned into five equivalent cubes. The reader may find the colored illustrations in DuVal's book [41] helpful in visualizing this particular construction.

Correspondences between I and A_5

The rotations of the point group I are now applied to the complete icosahedral set of five octahedra and the resulting permutations of the octahedra are observed. The identity operation E of I will clearly leave the octahedra unaffected and will therefore correspond to the A_5 cycle index term x_1^5. The rotations $12C_5$ and $12C_5^2$ of I will cyclically permute the five octahedra of the icosahedral set and thus correspond to the A_5 cycle index term $24x_5$. The rotations $20C_3$ of I will leave two of the octahedra fixed and cyclically permute the other three octahedra; they thus correspond to the A_5 cycle index term $20x_1^2x_3$. Similarly, the $15C_2$ of I will leave one octahedron fixed and interchange pairwise the other four, thereby corresponding to the A_5 cycle index term $15x_1x_2^2$. These observations thus lead to the following correspondences between the rotations of the point group I and the cycle index terms of the alternating group A_5:

$$E \to x_1^5 \tag{12}$$

$$12C_5 + 12C_5^2 \rightarrow 24x_5 \tag{13}$$

$$20C_3 \rightarrow 20x_1^2x_3 \tag{14}$$

$$15C_2 \rightarrow 15x_1x_2^2. \tag{15}$$

An alternative approach to the above procedure is to partition the 20 faces of an icosahedron into five sets of four faces, such that the midpoints of the four faces in each set from a regular tetrahedron. The relative positions of the corresponding five sets (each of four vertices) on a regular dodecahedron, the dual of the icosahedron, are indicated by the letters *A*, *B*, *C*, *D*, and *E* in Fig. 2, the Schlegel diagram of the regular dodecahedron. The permutations of these five tetrahedra under the rotations of the point group *I* correspond exactly to the permutations of the icosahedral set of five octahedra discussed above. These permutations thus lead to the same correspondences, given in Eqs. (12)–(15), between the rotations of the point group *I* and the cycle index terms of the alternating group A_5.

Unlike the regular icosahedron, a regular tetrahedron does not have an inversion center. Accordingly, inversion of any of the five tetrahedra of the icosahedral set will lead to a new tetrahedron which is the enantiomer of the original tetrahedron. The inverted tetrahedron is conveniently referred to as the *diametral tetrahedron.* Both a tetrahedron and its diametral tetrahedron cannot be members of the same icosahedral set of five tetrahedra. However, of interest is the fact that the eight vertices of a tetrahedron and its diametral tetrahedron form a cube. Furthermore, if the eight faces containing the vertices of this cube are subtracted from the 20 faces of the original icosahedron, the remaining 12 faces are exactly those which define an octahedron of the icosahedral set as outlined above. This relates to the observation that the cube formed by a tetrahedron and its diametral tetrahedron is the dual [24] of the octahedron. In this sense, the partitionings of an icosahedron into five tetrahedra and five octahedra are dual partitionings. Such partitionings should therefore yield identical correspondences to those in Eqs. (12)–(15) between the rotations of the point group *I* and the cycle index terms of the alternating group A_5.

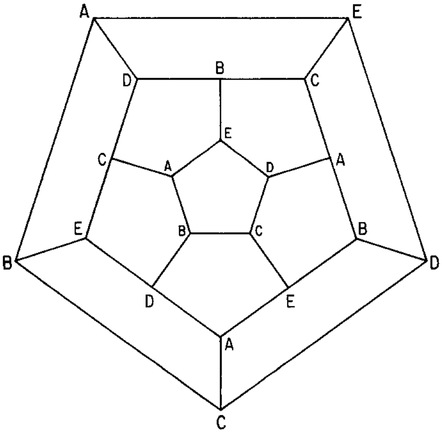

Fig. 2. The relative positions of the five sets of four vertices on a regular dodecahedron

The correspondence between the operations in the full icosahedral point group, I_h, and the symmetric group, S_5, can also be checked by procedures analogous to those given above using the icosahedral set of either five octahedra or five cubes, the latter arising from diametrically related tetrahedron pairs. In this instance, however, the improper rotations of I_h, namely i, $12S_{10}$, $12S_{10}^3$, $20S_6$, and 15σ, lead to the same cycle index terms x_1^5, $24x_5$, $20x_1^2x_3$, and $15x_1x_2^2$, respectively, as the corresponding proper rotations E, $12C_5$, $12C_5^2$, $20C_3$, and $15C_2$, respectively. Thus, when the pure rotational group I is expanded to the full point group I_h, the even operations of the alternating group A_5 will be repeated rather than supplemented by the odd permutations of five objects to give the full symmetric group S_5. For this reason, the regular icosahedron (or, with appropriate adjustments, its dual, the regular dodecahedron) can be used as a model for the even permutations of five objects, such as five ligands attached to some central atom, provided that these can be represented by the alternating group A_5. The regular icosahedron cannot, however, be employed to model the total of the even and odd permutations of five objects represented by the symmetric group S_5.

Finally, the symmetries (automorphism groups) of the Desargues-Levi [17] and Petersen [18] graphs can also be related to the symmetrical group S_5 by examination of their conjugacy classes. It then becomes immediately evident that the automorphism group of the Petersen graph is isomorphic with the symmetry group S_5 [18], and the automorphism group of the Desargues-Levi graph is isomorphic with the direct product group $S_5 \times S_2$. The use of these graphs as topological representations for rearrangements in five-coordinate ML_5 complexes [15-17] is then readily apparent.

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