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Chemical applications of topology and group theory

15. Representations of polyhedral isomerizations using Gale diagrams*

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Polyhedral isomerizations of the type $P_1 \rightarrow P_2 \rightarrow P_3$ are degenerate if P_1 is combinatorically equivalent to P_3 and planar if P_2 is a planar polygon. This paper systematizes degenerate non-planar isomerizations of 5- and 6-vertex polyhedra by using their Gale diagrams which are 1- and 2-dimensional, respectively. Using this method, it is trivial to show that all degenerate non-planar isomerizations of 5-vertex polyhedra can be formulated as sequences of Berry pseudorotation processes, i.e. the prototypical diamond-square-diamond (dsd) process. The Gale diagrams of the 7 combinatorically distinct 6-vertex polyhedra consist necessarily of points on the circumference of the unit circle as well as the center in the case of the pentagonal pyramid. Study of allowed motions of these points along the circumference of the unit circle in these Gale diagrams reveal 6 different types of single or multiple parallel dsd processes or closely related dsd′ or sds processes connecting these 7 combinatorically distinct 6-vertex polyhedra. In addition, a study of allowed motions of the points on the circumference of the Gale diagrams of the 6-vertex polyhedra through the center reveal 2 additional degenerate non-planar isomerization processes of 6-vertex polyhedra which involve pentagonal pyramid intermediates.

Key words: Topology—Gale diagrams—Polyhedral isomerizations—Diamond-square-diamond processes.

1. Introduction

Research during the past several years has led to a variety of approaches for the theoretical treatment of stereochemical non-rigidity in ML_n coordination complexes (M = central atom, generally a metal; L = ligands surrounding M). Thus,

* For part 14 of this series see reference [1].

possible isomerizations of ML_n polyhedra [$n = 4$ Ref. [2], 5 Ref. [3], 6 Ref. [4], and 8 Ref. [5]] have been represented topologically [2, 6] as graphs in which the vertices represent different polyhedral isomers and the edges represent possible one-step isomerizations. The individual polyhedral isomerizations have been described in terms of so-called diamond-square-diamond (dsd) processes [7]. In these terms the inherent fluxionality of polyhedra can be related to topological features which correspond to the ability of an individual polyhedron to isomerize to an equivalent polyhedron through a dsd process [8].

A question which is not clear from these and related theoretical studies is the extent to which *all* possible polyhedral isomerizations can be represented as dsd processes. The general impression from all of the theoretical work on polyhedral rearrangements is that specific polyhedra and specific polyhedral isomerization processes are selected without any attempt to determine all possible polyhedra and polyhedral isomerizations for a given coordination number. Actually from the chemical point of view, the first (and easier) half of this problem is essentially solved since all polyhedra having up to 8 vertices have been characterized [9] albeit as their duals [10] (i.e. polyhedra having no more than 8 faces). This paper presents a solution of the second half of the problem for polyhedra with 5 and 6 vertices by using Gale diagrams [10] to study all possible vertex motions in these polyhedra.

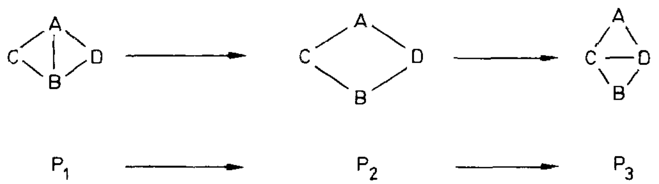
2. Background

Consider the polyhedron formed by the ligand donor atoms L in an ML_n coordination complex or the vertex atoms in a metal cluster, polyhedral borane, etc. Properties of such polyhedra which have been characterized in previous papers include their topologies [11] (vertex, edge, and face relationships) and symmetries (automorphism (point) groups [12] or chirality functions [13]). Polyhedra may also be characterized by their vertex plane structure. A *vertex plane* of a polyhedron is any plane containing 3 or more vertices of the polyhedron. All faces of the polyhedron are necessarily vertex planes. In addition, all polyhedra except the tetrahedron also have *non-facial* vertex planes, i.e. vertex planes which are not faces. The simplest example of a non-facial vertex plane is the plane formed by the 3 equatorial vertices of a trigonal bipyramid.

A minimum of 3 points is needed to define a plane. Therefore, a vertex plane containing only 3 vertices is an *ordinary vertex plane.* Special vertex planes, on the other hand, contain 4 or more vertices. Since a polyhedron with v vertices is by definition a 3-dimensional figure, no vertex planes in any polyhedron can contain all v vertices. A polyhedron with a necessarily facial vertex plane containing $v-1$ vertices is a pyramid. A polyhedron with a *non-facial* vertex plane containing $v-2$ vertices is a bipyramid.

A polyhedral isomerization step may be defined [6] as a deformation of a specific polyhedron P_1 to the point that the vertices define a new polyhedron P_2. Of particular interest in the context of this work are sequences of two polyhedral isomerization steps $P_1 \to P_2 \to P_3$ in which the polyhedron P_3 is combinatorically equivalent to the polyhedron P_1 (i.e. the "same" polyhedron) albeit with some permutation of the vertices not necessarily the identity permutation. A polyhedral isomerization sequence of the type $P_1 \to P_2 \to P_3$ in which P_1 and P_3 are combinatorically equivalent may be called a *degenerate polyhedral isomerization* with P_2 as the *intermediate polyhedron.* A degenerate polyhedral isomerization with a planar intermediate "polyhedron" (i.e. a polygon) may be called a *planar polyhedral isomerization.* The simplest example of a planar polyhedral isomerization is the interconversion of two tetrahedra (P_1 and P_3) through a square planar intermediate P_2. Except for this simplest example, planar polyhedral isomerizations are unfavorable owing to excessive intervertex repulsion and, in the case of ML_n coordination complexes, unfavorable or impossible hybridizations of the available M valence orbitals. The theoretical treatment in this paper is limited to the more interesting and more complicated non-planar polyhedral isomerizations $P_1 \to P_2 \to P_3$ in which the intermediate polyhedron P_2 is a true three-dimensional figure rather than a planar polygon.

The simplest example of a non-planar polyhedral isomerization is the Berry pseudorotation [14, 15] in which two trigonal bipyramidal isomers are interconverted through a square pyramid intermediate. This is also the simplest example of a dsd process which can be depicted schematically as follows:



A previous paper of this series [8] analyzes the topologies of deltahedra having minimum numbers of degree 3 vertices in terms of the presence of sites (called *dsd-situations*) which permit degenerate polyhedral isomerizations through dsd-processes.

Series and parallel combinations of dsd processes are possible. A pair of dsd processes in series involves a sequence of two dsd isomerizations $P_1 \to P_2 \to P_3 \to P_4 \to P_5$ in which $P_1 \to P_2 \to P_3$ and $P_3 \to P_4 \to P_5$ are separate dsd processes and P_1, P_3, and P_5 are combinatorically equivalent. If P_2 and P_4 are also combinatorically equivalent the sequence $P_2 \to P_3 \to P_4$ may be regarded as a square-diamond-square process (sds process). A degenerate sds process in the absence of degenerate dsd processes is also possible if in a sequence $P_1 \to P_2 \to P_3 \to P_4 \to P_5$ the polyhedra P_2 and P_4 are combinatorically equivalent and $P_1 \to P_2 \to P_3$ and/or $P_3 \to P_4 \to P_5$ are *non-degenerate* dsd processes (i.e. P_3 and P_1 and/or P_3 and P_5 are *not* combinatorically equivalent).

A pair of dsd processes in parallel involves two concerted dsd processes. A good example of such a double dsd process is the interconversion of two D_{2d}-dodecahedra through a square antiprismatic intermediate [5]. The interconversion of two octahedra through a trigonal prismatic intermediate [4] is an example of a triple dsd process (i.e. three dsd processes in parallel).

3. Gale diagrams

Studies of complex polytopes have benefited by use of their Gale diagrams [10] in cases where the dimensionality of the Gale diagram is less than that of the original polytope. As will be seen below, Gale diagrams of 5- and 6-vertex polyhedra can be imbedded into 1- and 2-dimensional space, respectively, thereby making them useful for the study of the isomerizations of such polyhedra.

In order to obtain a Gale diagram for a given polyhedron, the polyhedron is first subjected to a *Gale transformation.* Consider a polyhedron with v vertices as a set of v points $X_1, \ldots, X_v$ in 3-dimensional space R^3. These points may be regarded as 3-dimensional vectors $X_n = (x_{n,1}, x_{n,2}, x_{n,3})$, $1 \leq n \leq v$, from the origin to the polyhedron vertices. In addition, consider a set of points $D(A)$ in v-dimensional space R^v, $A = (a_1, \ldots, a_v)$ such that the following sums vanish:

$$\sum_{i=1}^{v} a_i x_{i,k} = 0 \quad \text{for } 1 \leq k \leq 3 \tag{1a}$$

$$\sum_{i=1}^{v} a_i = 0. \tag{1b}$$

Equation (1a) may also be viewed as 3 orthogonality relationships between the v-dimensional vector $A = (a_1, \ldots, a_v)$ and the three v-dimensional vectors $(x_{1,k}, x_{2,k}, \ldots, x_{v,k})$, $1 \leq k \leq 3$. Now consider the locations of the vertices of the polyhedron as the following $v \times 4$ matrix:

$$D_0 = \begin{pmatrix} x_{1,1} & x_{1,2} & x_{1,3} & 1 \\ x_{2,1} & x_{2,2} & x_{2,3} & 1 \\ \vdots & \vdots & \vdots & \vdots \\ x_{v,1} & x_{v,2} & x_{v,3} & 1 \end{pmatrix}. \tag{2}$$

Consider the columns of D_0 as vectors in R^v. Since D_0 has rank 4, the 4 columns of D_0 are linearly independent. Hence, the subspace $M(X)$ of R^v represented by these 4 linearly independent columns has dimension 4. Its orthogonal complement $M(A)^{\perp} = \{A \in R^v \mid A \cdot X = 0 \text{ for all } X \in M(X)\}$ coincides with $D(A)$ defined as above by Eqs. (1a) and (1b). Therefore:

$$\dim D(A) = \dim M(A)^{\perp} = v - \dim M(X) = v - 4. \tag{3}$$

Now define the following $v \times (v-4)$ matrix:

$$D_1 = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,v-4} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,v-4} \\ \vdots & \vdots & \cdots & \vdots \\ a_{v,1} & a_{v,2} & \cdots & a_{v,v-4} \end{pmatrix}. \tag{4}$$

The rows of D_1 may be considered as vectors in $v-4$ dimensional space; conventionally the jth row is denoted by $\bar{x}_j = (a_{j,,1}, a_{j,2}, \ldots, a_{j,v-4})$ for $j = 1, \ldots, v$.

The final result of this construction is the assignment of a point $\bar{x}_j$ in $v-4$ dimensional space (R^{v-4}) to each vertex x_j of the polyhedron. The collection of v points $\bar{x}_1, \ldots, \bar{x}_v$ in R^{v-4} is called a *Gale transform* of the set of vertices $x_1, \ldots, x_v$ of the polyhedron in question. The following features of a Gale transform of a polyhedron should be noted:
(1) A Gale transformation of two or more vertices of a polyhedron may lead to the same point $\bar{x}_j$, i.e. some points of a Gale transform may have a *multiplicity* greater than 1 so that the Gale transform of a polyhedron contains fewer *distinct* points than the polyhedron has vertices.
(2) The Gale transform depends upon the choice of the basis of the $M(A)^{\perp}$ subspace (e.g. the location of the origin in the coordinate system). Therefore, infinitely many Gale transforms are possible for a given polyhedron. Geometrically, a Gale transform of a polyhedron is a projection of the v vertices of a $v-1$ dimensional simplex (higher dimensional analogue of the tetrahedron) onto a $v-4$ dimensional hyperplane [16, 17]. Since infinitely many such projections are possible, the Gale transform for a given polyhedron is not unique.

In practice, it is easier to work with *Gale diagrams* corresponding to Gale transforms of interest. Condider a Gale transform of a polyhedron with v vertices $\bar{x}_1, \ldots, \bar{x}_v$ as defined above. The corresponding Gale diagram $\hat{x}_1, \ldots, \hat{x}_v$ is defined by the following relationships:[10]

$$\hat{x}_i = 0 \quad \text{if } \bar{x}_i = 0 \tag{5a}$$

$$\hat{x}_i = \frac{\bar{x}_i}{\|\bar{x}_i\|} \quad \text{if } \bar{x}_i \neq 0. \tag{5b}$$

In relationship (5b) $\|\bar{x}_i\|$ is the length of the vector $\bar{x}_i$ (i.e. $(a_{i,1}^2 + a_{i,2}^2 + \cdots + a_{i,v-4}^2)^{1/2}$). If $v-4=1$ (i.e. $v=5$), Gale diagrams can only contain the points of the straight line 0, 1, and -1 of varying multiplicities m_0, m_1, and m_{-1}, respectively, where $m_0 \geq 0$, $m_1 \geq 2$, and $m_{-1} \geq 2$. If $v-4=2$ (i.e. $v=6$) Gale diagrams can only contain the center and circumference of the unit circle. These two types of Gale diagrams are of interest in the context of this paper since they represent significant structural simplifications of the corresponding polyhedra.

The following properties of Gale diagrams are of interest since they impose important restrictions on configurations of points which can be Gale diagrams:
(1) The set of vertices of a polyhedron *not* forming a given face or edge of the polyhedron is called a *coface* of the polyhedron. The regular octahedron is unusual since all faces are also cofaces corresponding to the faces. The interior of the figure formed by connecting the vertices of a Gale diagram corresponding to a coface must contain the central point.
(2) A $v-5$ dimensional plane or hyperplane passing through the central point of the Gale diagram bisects the space of the Gale diagram into two halfspaces. Each such halfspace must contain at least two vertices (or one vertex of multiplicity

2) of the Gale diagram *not* including any vertices actually in the bisecting plane or hyperplane. Such a halfspace is called an *open* halfspace.
(3) The central point is a vertex of a Gale diagram if and only if the corresponding polyhedron is a pyramid. This central vertex corresponds to the apex of the pyramid which is the coface corresponding to the base of the pyramid.

Gale diagrams simplify problems involving polyhedra in cases where the dimension of the Gale diagram is less than that of the polyhedron. For this reason

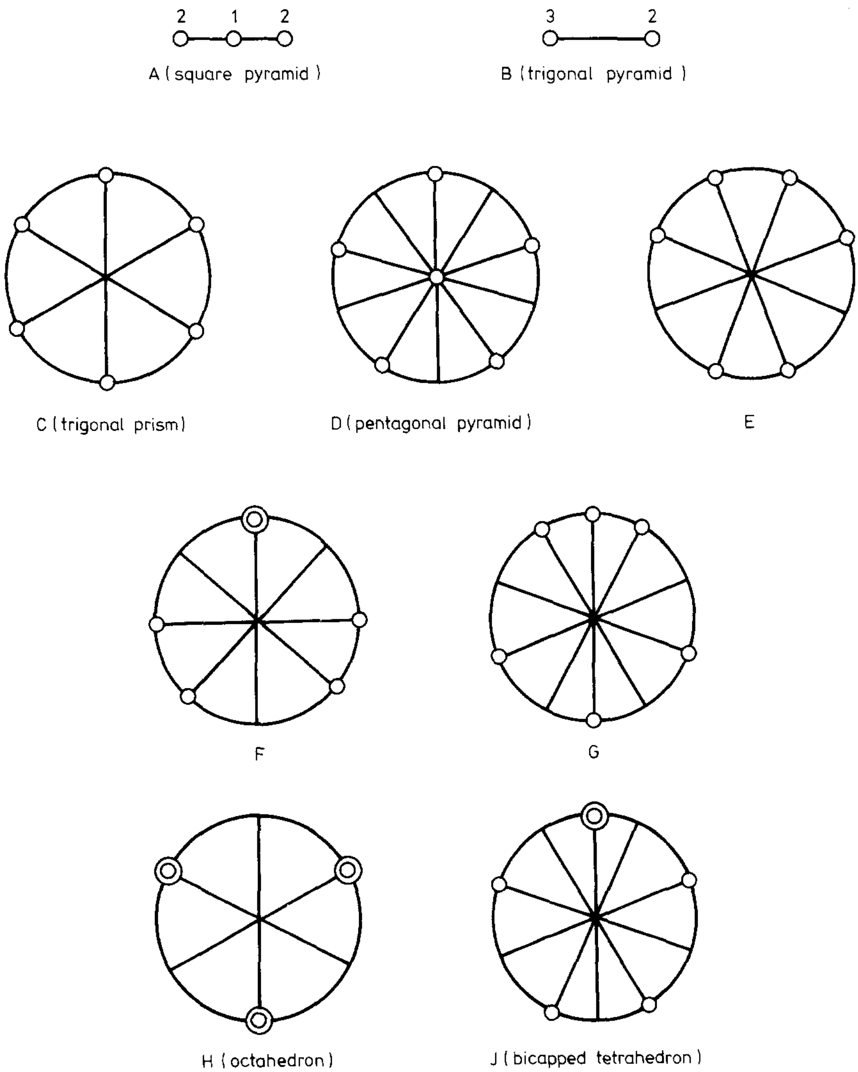


Fig. 1. Gale diagrams for the 2 combinatorially distinct 5-vertex polyhedra and the 7 combinatorially distinct 6-vertex polyhedra. The properties of these polyhedra are listed in Table 1. In the 6-vertex Gale diagrams vertices of multiplicity 1 are represented by a single circle and vertices of multiplicity 2 are represented by a double circle

Table 1. Properties of all possible five- and six-vertex polyhedra

Gale diagram[a]	Polyhedron name (if any)[b]	Edges	Faces	Symmetry[c]	Vertex types[d] v_3	v_4	v_5	Face types[e] f_3	f_4	f_5
A) Five-vertex polyhedra										
A	Square pyramid	8	5	C_{4v}	4	1	0	4	1	0
B	Trigonal bipyramid	9	6	D_{3h}	2	3	0	6	0	0
B) Six-vertex polyhedra										
C	Trigonal prism	9	5	D_{3h}	6	0	0	2	3	0
D	Pentagonal pyramid	10	6	C_{5v}	5	0	1	5	0	1
E	"Irregular hexahedron"	10	6	C_2	4	2	0	4	2	0
F	Diagonally deficient cube	11	7	C_{2v}	2	4	0	6	1	0
G		11	7	C_s	3	2	1	6	1	0
H	Octahedron	12	8	O_h	0	6	0	8	0	0
J	Bicapped tetrahedron	12	8	C_{2v}	2	2	2	8	0	0

[a] See Fig. 1 for these Gale diagrams.
[b] Polyhedra are named as in King, R. B. Ref. [16].
[c] The Schoenfliess point group notation is used as described in Cotton, F. A.: Chemical applications of group theory, New York: Interscience Publishers, 1963.
[d] The designations v_n refer to the numbers of vertices of degree n.
[e] The designations f_3, f_4, and f_5 refer to the numbers of faces which are triangles, quadrilaterals, and pentagons, respectively.

5- and 6-vertex polyhedra are effectively studied by using their Gale diagrams which have dimensions $(v-4)$ of 1 and 2, respectively. Figure 1 illustrates the Gale diagrams for the two 5-vertex polyhedra and seven 6-vertex polyhedra listed in Table 1. The remainder of this paper discusses non-planar polyhedral isomerizations of 5- and 6-vertex polyhedra in terms of allowed vertex motions in the corresponding Gale diagrams. In this context, an *allowed vertex motion* of a Gale diagram is a motion of one or more vertices which converts the Gale diagram of a polyhedron into that of another polyhedron with the same number of vertices without ever passing through an impossible Gale diagram such as one with an open halfspace containing only one vertex of unit multiplicity. Since two polyhedra are combinatorically equivalent if and only if their Gale diagrams are isomorphic [17], such allowed vertex motions of Gale diagrams are faithful representations of all possible non-planar polyhedral isomerizations.

4. Isomerizations of five-vertex polyhedra

The only possible 5-vertex polyhedra are the square pyramid and trigonal bipyramid. Their Gale diagrams (A and B, respectively, in Fig. 1) are the only 2 possible 1-dimensional 5-vertex Gale diagrams which have the required 2 vertices in each open half-space (i.e. m_1 and $m_{-1} \geq 2$). The only allowed vertex motion in a Gale diagram of a trigonal bipyramid involves motion of one point from the vertex of multiplicity 3 through the center point to the vertex originally of multiplicity 2. This interchanges the vertices of multiplicities 2 and 3 and leads to an equivalent Gale diagram corresponding to an isomeric trigonal bipyramid. The motion through the center point of the Gale diagram corresponds to the generation of a square pyramidal intermediate in the non-planar degenerate isomerization of a trigonal bipyramid. This, of course, is the Berry pseudorotation process [14, 15] which is the prototypical dsd process as discussed above. The choice of 3 points to move away from the vertex of multiplicity 3 in the Gale diagram of the trigonal bipyramid corresponds to the presence of 3 degenerate edges [8] in a trigonal bipyramid, where a *degenerate edge* is an edge which can be broken as the first step of a degenerate simple dsd polyhedral isomerization.

This analysis of the Gale diagrams of the 2 possible 5-vertex polyhedra shows clearly that the only possible non-planar isomerizations of 5-vertex polyhedra can be represented as successive dsd processes corresponding to successive Berry pseudorotations.

5. Isomerizations of six-vertex polyhedra

The Gale transforms of the vertex set of 6-vertex polyhedra are 2-dimensional $(v-4=2)$. The corresponding Gale diagrams (Fig. 1: C through J, inclusive) have vertices on the circumference of the unit circle. In addition, the center of the circle is a vertex of the Gale diagram for the pentagonal pyramid. The maximum multiplicity of a vertex in the Gale diagram of a 6-vertex polyhedron is 2 since otherwise there would be open halfspaces containing only one point (i.e. one of the open semicircles obtained by bisecting the unit circle using the diameter containing the vertex of multiplicity ≥ 3).

The Gale diagrams of 6-vertex polyhedra can be visualized most clearly if all of the diameters containing vertices are drawn as in Fig. 1. Some of these Gale diagrams can then be seen to have diameters with vertices of unit multiplicity at *each* end. Such diameters may be called *balanced diameters.* The two vertices of a balanced diameter form an edge which is a coface corresponding to a quadrilateral face of the polyhedron. Therefore, the number of balanced diameters in a Gale diagram of a 6-vertex polyhedron is equal to the number of quadrilateral faces of the polyhedron.

Polyhedral isomerizations in 6 vertex polyhedra may be represented by allowed motions of the vertices of their Gale diagrams along the circumference of the unit circle or through the center in the case of polyhedral isomerizations involving a pentagonal bipyramid intermediate. However, vertex motions are not allowed if at any time they generate one or more *forbidden diameters*, where a forbidden diameter is one containing 3 (or more) vertices. Forbidden diameters may be of one of the following 4 types:
D201: A vertex of multiplicity 1 at one end and one of multiplicity 2 at the other end.
D300: A vertex of multiplicity 3 at one end.
D111: A vertex of multiplicity 1 at each end and one of multiplicity 1 in the center.
D210: A vertex of multiplicity 2 at one end and one of multiplicity 1 in the center.

Each of these types of forbidden diameters bisects the unit circle of a 6-vertex Gale diagram into 2 open semicircles, one of which cannot contain the required 2 vertices since only 3 vertices of the 6 are left for both open semicircles.

Using these techniques all non-planar degenerate isomerizations involving 6-vertex polyhedra can be decomposed into sequences of the 8 fundamental processes listed in Table 2. These have the following essential properties:

(*1*) *Octahedron* (*H*)*–trigonal prism* (*C*)*–octahedron* (*H*). This triple dsd-process shows up as the Bailar Twist [18] and the Rây and Dutt Twist [19] in 6-coordinate chelates of the type M(bidentate)$_3$. Both of these processes involve the same type of rearrangement of the polyhedral vertices but have different types of edges in the trigonal prismatic intermediate bridged by the bidentate ligand.

(*2*) *Bicapped tetrahedron* (*J*)*–6, 11, 7-polyhedron* (*G*)*–bicapped tetrahedron*(*J*). This is the only possible *single* true dsd degenerate isomerization in 6-vertex deltahedra.

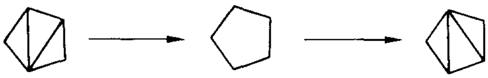
(*3*) *Bicapped tetrahedron* (*J*)*–pentagonal pyramid* (*D*)*–bicapped tetrahedron* (*J*). This is the simplest example of an isomerization involving simultaneous breaking of two edges of a deltahedron to form a pentagonal face followed by formation of two new edges to form an equivalent deltahedron. The action

Table 2. The 8 fundamental degenerate isomerization processes of six-vertex polyhedra

Process[a]	Process type[b]
$H \to C \to H$	3 dsd
$J \to G \to J$	dsd
$J \to D \to J$	5-pyramidal
$G \to E \to G$	dsd′
$G \to D \to G$	5-pyramidal
$F \to H \to F$	sds
$F \to E \to F$	dsd′
$E \to C \to E$	dsd or dsd′

[a] The polyhedra are designated by the letters used in Table 1.
[b] See text for a detailed discussion of these processes.

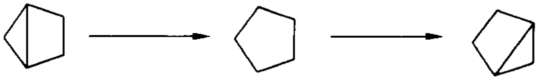
involving the pentagonal face of the pentagonal pyramid intermediate can be represented schematically as follows:



A process of this type can be called a *5-pyramidal process* since its simplest example (the process in question) involves interconversion of equivalent deltahedra through a pentagonal pyramid intermediate. Using this terminology, the dsd process can be called analogously a 4-pyramidal process since its simplest example (the Berry pseudorotation of the trigonal bipyramid $B \to A \to B$ discussed above) involves a square pyramid intermediate. Thus, in theory, each new number of vertices v can introduce a new $(v-1)$-pyramidal process. However, these processes rapidly become increasingly unfavorable in ML_n complexes as the number of vertices increases owing to the general unfavourability of large numbers of coplanar ligands L as discussed above in the context of planar polyhedral isomerizations.

(*4*) *G-E-G.* This process involving relatively non-descript low symmetry 6-vertex polyhedra looks like a dsd process but is not really one. Note that the 6,11,7-polyhedron G has one quadrilateral face. Rupture of one of the two edges of G connecting the vertex of degree 5 with one of degree 4 generates a new quadrilateral face to form E which has two quadrilateral faces. A new edge is then formed along the diagonal of the quadrilateral face of E corresponding to the *original* quadrilateral face of G and connecting a vertex of degree 4 with one of degree 3. An ordinary dsd process involves subtraction of an edge to convert two adjacent triangular faces into a quadrilateral face followed by addition of a new edge across the diagonal of this new quadrilateral face to convert this quadrilateral face back to two new triangular faces. In the modified dsd process *G-E-G* (called a dsd′ process) the quadrilateral face to which the diagonal edge is added is not the same as the quadrilateral face previously obtained after subtracting an edge connecting two triangular faces. Of course, the dsd′ process is only possible if the initial polyhedron contains at least one quadrilateral face.

(*5*) *G-D-G.* The unique edge e_{44} of the 6,11,7-polyhedron connecting the two vertices of degree 4 is removed to generate a pentagonal pyramid (after necessary vertex movements towards coplanarity of five vertices). In this way, the triangular and quadrilateral faces of G connected by e_{44} become the pentagonal base of the pentagonal pyramid (D). A new edge (different from e_{44}) is added across the pentagonal base of the pyramid to form a different pair of triangular and quadrilateral faces to give a different 6,11,7-polyhedron equivalent to G. The action involving the pentagonal face of the pentagonal pyramid can be represented schematically as follows:



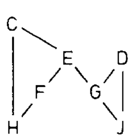
This process can be regarded as a 5-pyramidal process of a different type than the *J-D-J* process.

(*6*) *F-H-J*. This is an example of a square-diamond-square (sds) process which does not have a corresponding dsd process capable of degenerately isomerizing the polyhedron with the larger number of edges (in this case, the regular octahedron H). Thus addition to the 6,11,7-polyhedron of a single edge connecting the two vertices of degree 3 leads to a regular octahedron. Removal of any other of the 12 edges of this octahedron regenerates a 6,11,7-polyhedron F which is equivalent but not identical to the original 6,11,7-polyhedron. However, a regular octahedron cannot be converted to another regular octahedron through a single dsd process involving a 6,11,7-polyhedron F as an intermediate; such a process can only convert a regular octahedron to a bicapped tetrahedron, i.e. *H-F-J*. This relates to the earlier observation [8] that none of the 12 edges of the regular octahedron are degenerate. Furthermore, neither *J-F-J* nor *F-J-F* are fundamental degenerate isomerization processes since neither J nor F can undergo a simple degenerate isomerization through F or J intermediates, respectively, as can be shown by experimenting with their Gale diagrams.

(*7*) *F-E-F*. This is another example of dsd′ process discussed in detail above for the *G-E-G* process.

(*8*) *E-C-E*. This can be either a dsd or dsd′ process depending upon whether the edge added to the trigonal prism intermediate C is a diagonal of the new quadrilateral face generated by removal of the edge from the original 6,10,6-polyhedron E.

The relationships between the different 6-vertex polyhedra can be represented by the following *isomerization lattice* in which the 8 edges represent the pairs of polyhedra involved in the 8 fundamental non-planar degenerate isomerization processes noted above (the letters of the vertices refer to the designations of the polyhedra in Table 1):



Letters corresponding to 6-vertex polyhedra with the same numbers of edges (and faces) are depicted at the same level in this lattice. Similar isomerization lattices are likely to be useful for representing relationships between the sets of polyhedra with the same numbers of vertices v where $v>6$. The number of possible combinatorically distinct polyhedra increases rapidly as v increases above 6. Thus, the numbers of combinatorically distinct polyhedra with 7 and 8 vertices are 34 and 257, respectively [9]. Also, the Gale diagrams for polyhedra with 7 or more vertices require 3 or more dimensions (i.e. $v-4\geq 3$) and therefore are not useful for studying the isomerization of such polyhedra.

6. Conclusions

This paper shows how Gale diagrams are a useful device for studying isomerizations of polyhedra having so few vertices, namely 5 or 6, that the dimensionality of the Gale diagram is less than 3. Thus, this method provides a clear demonstration that isomerizations of 5-vertex polyhedra must involve either a planar pentagon intermediate or successive Berry pseudorotations [14, 15] (i.e. dsd processes). Isomerizations involving the seven 6-vertex polyhedra, of course, are considerably more complex. However, the use of Gale diagrams facilitates the search for the 8 fundamental non-planar isomerization processes of 6-vertex polyhedra (Table 2). Six of these 8 processes are single or multiple parallel dsd processes or the related dsd′ or sds processes. The remaining 2 processes involve pentagonal pyramid intermediates.

The Gale diagram approach does not appear to be advantageous for the direct study of isomerizations in polyhedra with more than 6 vertices since the corresponding Gale transformations do not reduce the dimensionality of the system. However, the analysis in this paper for 5- and 6-vertex polyhedra suggests that non-planar isomerizations in v-vertex polyhedra can be described as a series of p-pyramidal processes where $4\leq p\leq v-1$. Furthermore, p-pyramidal processes become increasingly less favorable with increasing p because of the larger number of required coplanar vertices for the p-pyramidal intermediate. This is consistent with an assumption in an earlier paper of this series [8] that the lowest energy processes for polyhedral rearrangements can be decomposed into one or more dsd processes.

References

1. King, R. B.: Theor. Chim. Acta (Berl.) **63**, 323 (1983)
2. Muetterties, E. L.: J. Am. Chem. Soc. **91**, 1636 (1969)
3. Brocas, J.: Top. Curr. Chem. **32**, 43 (1972)
4. Muetterties, E. L.: J. Am. Chem. Soc. **90**, 5097 (1968)
5. King, R. B.: Theor. Chim. Acta (Berl.) **59**, 25 (1981)
6. Klemperer, W. G.: J. Am. Chem. Soc. **94**, 6940 (1972)
7. Lipscomb, W. N.: Science **153**, 373 (1966)
8. King, R. B.: Inorg. Chim. Acta **49**, 237 (1981)
9. Federico, P. J.: Geom. Ded. **3**, 469 (1975)
10. Grünbaum, B.: Convex polytopes. New York: Interscience 1967

11. King, R. B.: J. Am. Chem. Soc. **91**, 7211 (1969)
12. King, R. B.: Inorg. Chem. **20**, 363 (1981)
13. King, R. B.: Theor. Chim. Acta (Berl.) **63**, 103 (1983)
14. Berry, R. S.: J. Chem. Phys. **32**, 933 (1960)
15. Holmes, R. R.: Accts. Chem. Res. **5**, 296 (1972)
16. McMullen, P., Shephard, G. C.: Mathematika **15**, 123 (1968)
17. McMullen, P., Shephard, G. C.: Convex polytopes and the upper bound conjecture. Cambridge: Cambridge University Press 1971
18. Bailar, J. C., Jr.: J. Inorg. Nucl. Chem. **8**, 165 (1958)
19. Ray, P., Dutt, N. K.: J. Inorg. Nucl. Chem. Soc. **20**, 81 (1943)

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