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# Symmetry Factoring of the Characteristic Equations of Graphs Corresponding to Polyhedra

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A systematic procedure is described which uses two-and three-fold symmetry elements in graphs to reduce their adjacency matrices to lead to corresponding factorings of their characteristic polynomials. A graph splitting algorithm based on this matrix reduction procedure is described. Applications of these methods to the factoring of the characteristic polynomials of 28 polyhedra with nine or less vertices are given. General expressions for the eigenvalues of prisms, pyramids, and bipyramids in terms of the eigenvalues of their basal or equatorial regular polygons are calculated by closely related matrix methods.

**Key words**: Graph theory – Graphs corresponding to polyhedra

## 1. Introduction

A fundamental understanding of the properties of three-dimensional polyhedra is important for structural chemistry. The spectra of such polyhedra as determined by solutions of the characteristic equations of their adjacency matrices [1] are related to interactions between atoms located at the vertices of the polyhedra and therefore are essential to the understanding of chemical systems. During the past several years I have investigated the properties of chemically significant polyhedra [2–6]. More recently, I have studied their eigenvalue patterns in attempts to relate these patterns to the energies of available atomic orbitals. During the course of this more recent work I have developed efficient and systematic procedures for using elements of symmetry in graphs for factoring their characteristic equations thereby facilitating determination of their eigenvalues and providing insight into effects of certain structural changes in certain graphs on their eigenvalue patterns. These new procedures thus provide a simple method for deriving general expressions for the eigenvalues of certain common families of polyhedra such as prisms, pyramids, and bipyramids.

This expository paper summarizes the highlights of these new matrix reduction and graph splitting procedures and illustrates their applications for the determination of characteristic equations of polyhedra with some symmetry but insufficient symmetry for many of the more powerful techniques of algebraic graph theory [1]. This paper first justifies these new techniques in terms of standard matrix theory [7, 8]. It then presents details of the corresponding graph splitting algorithm, which uses symmetry elements to convert a connected graph $G$ with $v$ vertices to a disconnected graph $G^*$ also with $v$ vertices but with $c$ components $G_1, \ldots, G_c$ such that the eigenvalues of $G^*$ are the same as those of $G$. However, whereas determination of the eigenvalues of $G$ requires solution of an equation of order $v$, determination of the equivalent eigenvalues of $G^*$ requires solution of equations of a lower degree $u$ where $u$ is the number of vertices in the largest component of $G^*$. Even if $G$ is the usual type of graph with all edges of unit weight in both directions, the corresponding graph $G^*$ arising from this graph reduction algorithm will have edges of variable and non-unit weights, different weights in each direction, and/or loops. However, the complications added by introduction of these features into $G^*$ from $G$ are far less than the simplifications in the expansion of the adjacency matrix into the characteristic polynomial and the reduction of the maximum degree of the equations that must be solved to obtain the eigenvalues.

## 2. A Matrix Description of the Procedure

Consider graph $G$ containing $v$ vertices with a two-fold symmetry element $s_2$ such that for the corresponding symmetry operation $s_2^2 = E$ where $E$ is the identity. Label as $z_1, \ldots, z_p$ the $p$ vertices of $G$ that are fixed under the symmetry operation $s_2$ (i.e. $s_2(z_i) = z_i$). Label as $a_1, \ldots, a_q$ the $q$ vertices of $G$ that transform under $s_2$ to $b_1, \ldots, b_q$, respectively. Then $p + 2q = v$. Furthermore, any pair $a_i, b_i$ is in the same orbit of the symmetry operation $s_2$. Consider the adjacency matrix $A(G)$ as formed by the following 9 submatrices:

$$\begin{pmatrix} A_{z,z} & A_{z,a} & A_{z,b} \\ A_{a,z} & A_{a,a} & A_{a,b} \\ A_{b,z} & A_{b,a} & A_{b,b} \end{pmatrix}.$$

If a similarity transformation $P^{-1}AP$ on $A(G)$ can be found such that the submatrices in the positions of $A_{b,z}$ and $A_{b,a}$, the positions of $A_{z,b}$ and $A_{a,b}$, or other adjacent non-diagonal positions become zero, then the problem of determining the eigenvalues of the $v \times v$ matrix $A$ can be reduced to the simpler problem of determining the eigenvalues of one $(p+q) \times (p+q)$ matrix and one $q \times q$ matrix where $p + 2q = v$.

Consider the following sequence of two steps:

1) Add to each column of $A$ corresponding to the vertex $a_i$ the column corresponding to the vertex $b_i$ in the same orbit of $s_2$ thereby leading to a new $v \times v$ matrix $A'$ which can be represented as

$$\begin{pmatrix} A_{z,z} & A_{z,a} + A_{z,b} & A_{z,b} \\ A_{a,z} & A_{a,a} + A_{a,b} & A_{a,b} \\ A_{b,z} & A_{b,a} + A_{b,b} & A_{b,b} \end{pmatrix}.$$

2) In the new matrix $A$ subtract from each row corresponding to the vertex $b_i$ the row corresponding to the vertex $a_i$ in the same orbit of $s_2$ leading to a third $v \times v$ matrix $A''$ which can be represented as

$$\begin{pmatrix} A_{z,z} & A_{z,a} + A_{z,b} & A_{z,b} \\ A_{a,z} & A_{a,a} + A_{a,b} & A_{a,b} \\ A_{b,z} - A_{a,z} & A_{b,a} + A_{b,b} - A_{a,a} - A_{a,b} & A_{b,b} - A_{a,b} \end{pmatrix}.$$

Step 1 above generates columns corresponding to each orbit of graph $G$ under symmetry operation $s_2$ (i.e. the columns of the types $A_{x,z}$ and $A_{x,a} + A_{x,b}$ where $x$ is $z$, $a$, or $b$). Step 2 involves taking the differences between pairs of rows corresponding to pairs of vertices in the same orbit. However, pairs of vertices $a_i$, $b_i$ in the same orbit of $G$ under $s_2$ will be equivalently situated with respect to all of the other orbits of $G$ under $s_2$ regardless of whether such orbits contain one vertex (i.e. $z_j$) or two vertices (i.e. $a_j$, $b_j$). For this reason clearly related to the presence of the symmetry element $s_2$ in $G$, the submatrices $A_{b,z} - A_{a,z}$ and $A_{b,a} + A_{b,b} - A_{a,a} - A_{a,b}$ will be zero indicating that $A''$ has the form

$$\begin{pmatrix} A_{z,z} & A_{z,a} + A_{z,b} & A_{z,b} \\ A_{a,z} & A_{a,a} + A_{a,b} & A_{a,b} \\ 0 & 0 & A_{b,b} - A_{a,b} \end{pmatrix}.$$

Consider the two $v \times v$ matrices $\boldsymbol{P}$ and $\boldsymbol{Q}$ such that $A\boldsymbol{P} = A'$ and $\boldsymbol{Q}A' = A''$. If $\boldsymbol{Q} = \boldsymbol{P}^{-1}$, then $A'' = \boldsymbol{P}^{-1} A\boldsymbol{P}$ and the two steps indicated above constitute a similarity transformation such that $\det(\lambda I - A) = \det(\lambda I - A'')$ thereby indicating that the eigenvalues of $A$ are identical to those of $A''$. More significantly, the location of the zero submatrices in $A''$ means that the eigenvalues of $A''$ will be identical to the eigenvalues of the smaller matrices[1]

$$\begin{pmatrix} A_{z,z} & A_{z,a} + A_{z,b} \\ A_{a,z} & A_{a,a} + A_{a,b} \end{pmatrix} \quad \text{and} \quad (A_{b,b} - A_{a,b}).$$

For convenience and future reference label these submatrices $A_g$ and $A_u$ respectively. Note that $A_g$ is a $(p + q) \times (p + q)$ matrix and $A_u$ is a $q \times q$ matrix.

The nature of step 1 means that $\boldsymbol{P}$ has the following form:

a) $p_{xx} = +1$ (diagonal elements);
b) $p_{xy} = +1$ and $p_{yx} = 0$ if $x$ is the row corresponding to any vertex $b_i$ and $y$ is the column corresponding to the vertex $a_i$($a_i$ and $b_i$ are in the same orbit under $s_2$);
c) all other $p_{mn} = 0$.

The nature of step 2 means that $\boldsymbol{Q}$ has the following form:

a) $q_{xx} = +1$ (diagonal elements);
b) $q_{xy} = -1$ and $q_{yx} = 0$ if $x$ is the row corresponding to any vertex $b_i$ and $y$ is the column corresponding to the vertex $a_i$($a_i$ and $b_i$ are in the same orbit under $s_2$);
c) all other $q_{mn} = 0$.

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[1] See Theorem 1, page 109 in [7] regarding a similar property in closely related triangular matrices.

The matrices $\boldsymbol{P}$ and $\boldsymbol{Q}$ are both unit lower triangular matrices. The non-diagonal entries of +1 in $\boldsymbol{P}$ are in identical positions to the corresponding non-diagonal entries of $-1$ in $\boldsymbol{Q}$. Therefore by the standard rules of matrix multiplication $\boldsymbol{PQ} = \boldsymbol{I}$ and $\boldsymbol{Q} = \boldsymbol{P}^{-1}$. Note that the appearance of the off-diagonal +1 entries in $\boldsymbol{P}$ in the same places as the off-diagonal $-1$ entries in $\boldsymbol{Q}$ is a strict requirement for $\boldsymbol{PQ} = \boldsymbol{I}$ and therefore for equivalence of the eigenvalues of $A''$ and $A$.

A variation of this type of procedure can be used for three-fold symmetry elements. Consider a graph $G$ with a three-fold symmetry element $s_3$ such that for the corresponding symmetry operation $s_3^3 = E$ (i.e. a three-fold rotation axis). Label as $z_1, \ldots, z_p$ the $p$ vertices that are fixed under $s_3$ (i.e. lie on the three-fold rotation axis so that $s_3(z_i) = z_i$). Label as $a_1, \ldots, a_q, b_1, \ldots, b_q$, and $c_1, \ldots, c_q$ the three sets of $q$ vertices of $G$ such that $s_3(a_i) = b_i$ and $s_3^2(a_i) = c_i$ for $1 \leqslant i \leqslant q$. Thus $p + 3q = v$ and the vertices of any triplet $a_i, b_i, c_i$ $(1 \leqslant i \leqslant q)$ are in the same orbit of the symmetry operation $s_3$.

Consider the adjacency matrix $A(G)$ as formed by the following 16 submatrices:

$$\begin{pmatrix} A_{z,z} & A_{z,a} & A_{z,b} & A_{z,c} \\ A_{a,z} & A_{a,a} & A_{a,b} & A_{a,c} \\ A_{b,z} & A_{b,a} & A_{b,b} & A_{b,c} \\ A_{c,z} & A_{c,a} & A_{c,b} & A_{c,c} \end{pmatrix}.$$

Consider the following sequence of two steps analogous to those for the two-fold symmetry element $s_2$ discussed above:

1) Add to each column corresponding to the vertex $a_i$ the columns corresponding to the vertices $b_i$ and $c_i$ in the same orbit leading to a new $v \times v$ matrix $A'$ which can be represented as

$$\begin{pmatrix} A_{z,z} & A_{z,a} + A_{z,b} + A_{z,c} & A_{z,b} & A_{z,c} \\ A_{a,z} & A_{a,a} + A_{a,b} + A_{a,c} & A_{a,b} & A_{a,c} \\ A_{b,z} & A_{b,a} + A_{b,b} + A_{b,c} & A_{b,b} & A_{b,c} \\ A_{c,z} & A_{c,a} + A_{c,b} + A_{c,c} & A_{c,b} & A_{c,c} \end{pmatrix}.$$

2) In the new matrix $A'$ subtract from each row corresponding to the vertices $b_i$ and $c_i$ the row corresponding to the vertex $a_i$ in the same orbit leading to a third $v \times v$ matrix $A''$ which can be represented as

$$\begin{pmatrix} A_{z,z} & A_{z,a} + A_{z,b} + A_{z,c} & A_{z,b} & A_{z,c} \\ A_{a,z} & A_{a,a} + A_{a,b} + A_{a,c} & A_{a,b} & A_{a,c} \\ A_{b,z} - A_{a,z} & A_{b,a} + A_{b,b} + A_{b,c} - A_{a,a} - A_{a,b} - A_{a,c} & A_{b,b} - A_{a,b} & A_{b,c} - A_{a,c} \\ A_{c,z} - A_{a,z} & A_{c,a} + A_{c,b} + A_{c,c} - A_{a,a} - A_{a,b} - A_{a,c} & A_{c,b} - A_{a,b} & A_{c,c} - A_{a,c} \end{pmatrix}$$

However, the submatrices $(A_{b,z} - A_{a,z})$, $(A_{b,a} + A_{b,b} + A_{b,c} - A_{a,a} - A_{a,b} - A_{a,c})$, $(A_{c,z} - A_{a,z})$, and $(A_{c,a} + A_{c,b} + A_{c,c} - A_{a,a} - A_{a,b} - A_{a,c})$ will all be zero since they arise from differences between rows corresponding to vertices in the same orbit of $G$ under $s_3$. Also the nature of the three-fold symmetry element will make any $b_i$ and $a_i$ situated equivalently relative to the corresponding $c_i$ and any $c_i$ and $a_i$ situated equivalently relative to the corresponding $b_i$ thereby making zero the submatrices $(A_{c,b} - A_{a,b})$ and $(A_{b,c} - A_{a,c})$. Therefore $A''$ has the form

$$\begin{pmatrix} A_{z,z} & A_{z,a} + A_{z,b} + A_{z,c} & A_{z,b} & A_{z,c} \\ A_{a,z} & A_{a,a} + A_{a,b} + A_{a,c} & A_{a,b} & A_{a,c} \\ 0 & 0 & A_{b,b} - A_{a,b} & 0 \\ 0 & 0 & 0 & A_{c,c} - A_{a,c} \end{pmatrix}.$$

This makes the eigenvalues of $A''$ identical to the eigenvalues of the smaller matrices

$$\begin{pmatrix} A_{z,z} & A_{z,a} + A_{z,b} + A_{z,c} \\ A_{a,z} & A_{a,a} + A_{a,b} + A_{a,c} \end{pmatrix} = A_a \qquad \begin{matrix} (A_{b,b} - A_{a,b}) = A_{e1} \\ (A_{c,c} - A_{a,c}) = A_{e2} \end{matrix}$$

again considerably simplifying the eigenvalue calculation problem.

In this case the eigenvalue calculation can be simplified still further. The nature of the three-fold symmetry operation $s_3$ on the graph $G$ requires that $b_i$ and $c_i$ be equivalently situated relative to $a_i$. Therefore just as $(A_{c,b} - A_{a,b}) = (A_{b,c} - A_{a,c}) = 0$ as discussed above so does also $(A_{b,b} - A_{a,b}) = A_{e1} = (A_{c,c} - A_{a,c}) = A_{e2} = A_e$. Thus the eigenvalues of $A''$ can be obtained from the eigenvalues of the two submatrices $A_a$ and $A_e$ with each eigenvalue of $A_e$ appearing twice as an eigenvalue of $A''$. Eigenvalues of $A_e$ of multiplicity $m$ will have multiplicity $2m$ as eigenvalues of $A''$.

It remains to be shown that the sequence of two steps outlined above for a graph $G$ containing a three-fold symmetry element $s_3$ leading from the adjacency matrix $A$ to $A''$ constitutes a similarity transformation such that the eigenvalues of $A''$ are the same as those of $A$. Consider the two $v \times v$ matrices $\boldsymbol{P}$ and $\boldsymbol{Q}$ such that $\boldsymbol{AP} = A'$ and $\boldsymbol{Q}A' = A''$. The nature of step 1 means that $\boldsymbol{P}$ has the following form:

a) $p_{xx} = +1$ (diagonal elements);
b) $p_{xy} = +1$ and $p_{yx} = 0$ if $y$ is the column corresponding to any vertex $a_i$ and $x$ is the row corresponding to the vertices $b_i$ or $c_i$ where $a_i$, $b_i$, and $c_i$ are all in the same orbit under the three-fold symmetry operation $s_3$;
c) all other $p_{mn} = 0$.

The nature of step 2 means that $\boldsymbol{Q}$ has the following form:

a) $q_{xx} = +1$ (diagonal elements);
b) $q_{xy} = -1$ and $q_{yx} = 0$ if $y$ is the column corresponding to any vertex $a_i$ and $x$ is the row corresponding to the vertices $b_i$ or $c_i$ where $a_i$, $b_i$, and $c_i$ are all in the same orbit under the three-fold symmetry operation $s_3$;
c) all other $q_{mn} = 0$.

Again $\boldsymbol{P}$ and $\boldsymbol{Q}$ are both unit lower triangular matrices. The non-diagonal entries of +1 in $\boldsymbol{P}$ are in identical positions to the corresponding non-diagonal entries of $-1$ in $\boldsymbol{Q}$. Therefore $\boldsymbol{PQ} = \boldsymbol{I}$ and $\boldsymbol{Q} = \boldsymbol{P}^{-1}$. This indicates that the two-step sequence above for the three-fold symmetry element $s_3$ constitutes a similarity transformation such that the eigenvalues of $A''$ are the same as those of $A$.

If the graph $G$ has several two- or three-fold symmetry elements then the procedures outlined above can be repeated for the different symmetry elements to reduce the matrix to the maximum possible extent thereby minimizing the degrees of the resulting factors of the characteristic polynomial of $G$. In the successive application of this procedure the sets of vertices remaining fixed under each of the symmetry operations used for the matrix reduction will be different. Therefore it will be necessary to transpose some of the rows and columns of the partially reduced matrix obtained after performing the complete two-step reduction procedure outlined above for two- and three-fold symmetry elements before proceeding with further matrix reduction using the next symmetry element. If done carefully, this constitutes a mere relabelling of the rows and columns of the partially reduced matrix without affecting the determinant and hence keeping unchanged the eigenvalues. The elements on the diagonal of the partially reduced matrix must remain on the diagonal on any such transposed matrix, i.e. rows and columns must be transposed equivalently. If this important precaution is not taken the procedures outlined above become invalid and meaningless.

Procedures similar to those outlined above can be derived for four- and higher-fold symmetry elements. The procedures will work completely analogously for a graph with an automorphism group [1, 9] of sufficiently high order and appropriate structure that the alternating group $A_n$ [10] can be a subgroup of the graph automorphism group. Thus the adjacency matrix of a cube can be reduced by first using a four-fold symmetry element corresponding to the alternating group $A_4$, which is a subgroup of the $O_h$ point group [11] of the cube. The details of the matrix reduction procedure using $A_4$ rather than $A_3$ (i.e. $s_3$ in the notation above) are completely analogous to those given above for the three-fold symmetry operation $s_3$ except in step 1 four rather than three columns corresponding to vertices in the same orbit are added together and in step 2 the row corresponding to the vertex whose column is the sum of the four columns of the vertices in the same orbit under $A_4$ is subtracted from three rather than two other rows of vertices in the same orbit under $A_4$. However, very few of the planar graphs corresponding to three-dimensional polyhedra are of such high symmetry that $A_n (n \geqslant 4)$ is a subgroup of their automorphism groups. Therefore the details of using $n$-fold symmetry elements $A_n (n \geqslant 4)$ to reduce the adjacency matrixes of graphs corresponding to three-dimensional polyhedra are unimportant and will not be discussed further in this paper.

Another type of $n$-fold symmetry element is the $n$-fold rotation axis $C_n$. For $n \neq 3$, $C_n \neq A_n$ since $C_n$ has $n$ operations whereas $A_n$ has $n!/2$ operations. A matrix reduction procedure for an $n$-fold symmetry element $C_n$ completely identical to that suggested above for $A_n$ is completely valid in that such a reduction procedure constitutes a similarity transformation such that the eigenvalues of the reduced matrix $A''$ will be the same as those of the original matrix $A$. However, the lower symmetry implied by $C_n$ relative to $A_n$ means that fewer of the submatrices in the reduced adjacency matrix will vanish making matrix reduction by a $C_n$ less effective at reducing the degrees of the factors of the characteristic polynomial than a matrix reduction by the corresponding $A_n$. Matrix reduction through an $n$-fold rotation axis $C_n$ is used later in this paper to derive general expressions for the eigenvalues of prisms, pyramids, and bipyramids. This later discussion can therefore serve an an illustration on generalizing the matrix reduction procedure detailed above for two- and three-fold symmetry operations to higher $n$-fold symmetry operations, specifically $n$-fold rotation axes.

## 3. A Graph Splitting Algorithm for Working the Above Matrix Procedure

The matrix reduction procedure outlined above for the adjacency matrix of a graph containing one or more two- or three-fold symmetry elements can be translated directly into corresponding operations on the graph itself. The result of the operations on the graph is to transform a connected graph $G$ with $v$ vertices by splitting into a disconnected graph $G''$ with $c$ components such that the set of eigenvalues of all of the components of the disconnected graph $G''$ is identical to the eigenvalues of the original connected graph $G$. However, determination of the eigenvalues of the disconnected graph $G''$ is considerably easier than the determination of the eigenvalues of the original connected graph $G$ for the following reasons:

1) The expansion of the determinant det $(\lambda I - A)$ to determine the characteristic equation of a connected graph $G$ with $v$ vertices in terms of sesquivalent edge-subgraphs [1, 12] rapidly becomes more difficult and less reliable as the number of vertices in $G$ is increased. If $G$ is reduced to a disconnected graph $G''$, the characteristic equation of each component $G_i''$ of this disconnected graph with $v_i$ vertices ($\Sigma_{i=1}^{c} v_i = v$) can be determined individually by the sesquivalent edge-subgraph procedure thereby decreasing considerably the sizes of sesquivalent edge-subgraphs that must be considered.
2) The degree of the equation that must be solved to determine the eigenvalues of the original connected graph $G$ with $v$ vertices is $v$ whereas the degrees of the equations that must be solved to determine the eigenvalues of the corresponding disconnected graph $G''$ are $v_1, \ldots, v_c$ such that $\Sigma_{i=1}^{c} v_i = v$. It is less difficult to solve $n$ different equations of degree $m$ than to solve a single equation of degree $mn$. Even a non-factorable cubic equation obtained as the characteristic equation of a three-vertex graph with unequal edge weights has no true algebraic solution [13] because of difficulties associated with the real cube roots of complex numbers with imaginary components.

Details of the graph splitting algorithm for both two- and three-fold symmetry elements are given below:

### *3.1. Two-Fold Symmetry Elements*

Consider a connected graph $G$ with $v$ vertices containing a two-fold symmetry element $s_2$ fixing the $p$ vertices $z_1, \ldots, z_p$ and transforming the $a_1, \ldots, a_q$ vertices of $G$ into the corresponding $b_1, \ldots, b_q$ vertices; $p + 2q = v$, the number of vertices of $G$

Convert the connected graph $G$ to a disconnected graph $G^*$ containing two components $G_g$ and $G_u$. $G_g$ and $G_u$ are both directed graphs (digraphs) with the following characteristics:

1) The edge weights are not necessarily unity as in a usual graph.
2) The weight of the edge connecting any two vertices $v_x$ and $v_y$ of either $G_g$ or $G_u$ is not necessarily equivalent in the two directions.
3) Either $G_g$, $G_u$, or both can contain loops not necessarily of unit weight. Let $w(a, b)$ be the weight of the edge connecting vertices $a$ and $b$ in $G$; when the edge $(a, b)$ involved is clear from the discussion, $w(a, b)$ will be abbreviated to $w$.

The component $G_g$ is the orbit graph of $G$ relative to the symmetry operation $s_2$ and has $p + q$ vertices corresponding to $z_1, \ldots, z_p$ and the identified pairs $(a_1, b_1), \ldots, (a_q, b_q)$. The edges of $G_g$ arise from those of $G$ as follows:

($G1$) An edge connecting $z_i$ and $z_j$ or $a_i$ and $a_j$ (and therefore $b_i$ and $b_j$ because of the presence of the symmetry element $s_2$) in $G$ will have the same weight in both directions and the same weight in $G_g$ as in $G$.
($G2$) Edges connecting $z_i$ with $a_j$ and $b_j$ of weight $w$ in $G$ will have weight $2w$ directed from $z_i$ towards $(a_j, b_j)$ and weight $w$ from $(a_j b_j)$ towards $z_i$ in $G_g$ where $(a_j, b_j)$ is the vertex corresponding to the identified pair $a_j$ and $b_j$.
($G3$) Edges connecting $a_i$ with $b_i$ of weight $w$ in $G$ will appear as a loop of weight $w$ attached to the vertex $(a_j, b_i)$ in $G_g$.
($G4$) Edges connecting $a_i$ with $b_j$ $(i \neq j)$ of weight $w$ in $G$ will connect the vertices $(a_i, b_i)$ and $(a_j, b_j)$ in $G_g$ with weight $w$ in each direction.

The adjacency matrix of $G_g$ corresponds to the submatrix $A_g$ in the matrix reduction procedure outlined above.

The component $G_u$ has $q$ vertices corresponding to the identified pairs $(a_1, b_1), \ldots, (a_q, b_q)$. The vertices corresponding to $z_1, \ldots, z_p$ in $G$ vanish in $G_u$. The edges in $G_u$ arise from those of $G$ as follows:

($U1$) Edges of the following types in $G$ vanish completely in $G_u$:
  a) Edges connecting $z_i$ and $z_j$ in $G$;
  b) Edges connecting $z_i$ with $a_j$ and $b_j$ in $G$.
($U2$) Edges connecting $a_i$ and $a_j$ in $G$ of weight $w$ (and therefore also connecting $b_i$ and $b_j$ because of the presence of the symmetry element $s_2$) will appear as edges between the vertices $(a_i, b_i)$ and $(a_j, b_j)$ in $G_u$ with weight $w$ in each direction.
($U3$) Edges connecting $a_i$ with $b_i$ of weight $w$ in $G$ will appear as a loop of weight $-w$ attached to the vertex $(a_i, b_i)$ in $G_u$.
($U4$) Edges connecting $a_i$ with $b_j (i \neq j)$ of weight $w$ in $G$ will connect the vertices $(a_i, b_i)$ and $(a_j, b_j)$ in $G_u$ with weight $-w$ in each direction.

The adjacency matrix of $G_u$ corresponds to the submatrix $A_u$ in the matrix reduction procedure outlined above.

The combined eigenvalues of the two components of $G^*$ ($G_g$ and $G_u$) as defined above will be the eigenvalues of the original connected graph $G$ since this graph reduction procedure corresponds to the matrix reduction procedure outlined above. Thus the graphs $G_g$ and $G_u$ have the adjacency matrices $A_g$ and $A_u$, respectively; the combined eigenvalues of $A_g$ and $A_u$ are the same as those of $A''$; and the eigenvalues of $A''$ are the same as those of $A$, the adjacency matrix of $G$.

### *3.2. Three-Fold Symmetry Operations*

Consider a connected graph $G$ with $v$ vertices $z_1, \ldots, z_p, a_1, \ldots, a_q, b_1, \ldots, b_q, c_1, \ldots, c_q, p + 3q = v$, and with a three-fold symmetry element $s_3$ (i.e. 3-fold rotation axis) such that $s_3(z_i) = z_i$ (i.e. $s_3$ fixes all $z_i$ - each $z_i$ lies on the 3-fold rotation axis), $s_3(a_i) = b_i$, and $s_3^2(a_i) = c_i$ for all $i$.

Convert the connected graph $G$ into a disconnected graph $G^*$ containing three components $G_a$, $G_e$, and $G_e$ of which the last two components $G_e$ are identical. Again $G_a$ and $G_e$ are digraphs similar to $G_g$ and $G_u$ for the analogous procedure involving two-fold symmetry elements discussed above. Again let $w(x, y)$ or more briefly $w$ denote the weight of the edge connecting the vertices $x$ and $y$ in $G$.

The component $G_a$ is the orbit graph of $G$ relative to $s_3$ and has $p + q$ vertices corresponding to $z_1, \ldots, z_p$ and the identified triplets $(a_1, b_1, c_1), \ldots, (a_q, b_q, c_q)$. The edges of $G_a$ arise from those of $G$ as follows:

($A1$) An edge connecting $z_i$ and $z_j$ or $a_i$ and $a_j$ (and therefore $b_i$ and $b_j$ as well as $c_i$ and $c_j$ in the latter case because of the presence of the three-fold symmetry element $s_3$) of weight $w$ in $G$ will have weight $w$ in each direction in $G_a$.

($A2$) Edges connecting $z_i$ with $a_j$, $b_j$, and $c_j$ in $G$ each of weight $w$ will have weight $3w$ directed from $z_i$ towards $(a_j, b_j, c_j)$ and weight $w$ directed from $(a_j, b_j, c_j)$ towards $z_i$ in $G_a$ where $(a_j, b_j, c_j)$ is the vertex corresponding to the identified triplet $a_j$, $b_j$, and $c_j$.

($A3$) The three edges of a triangle $a_ib_ic_i$ of weight $w$ in $G$ will appear as a loop of weight $2w$ attached to the vertex $(a_i, b_i, c_i)$ in $G_a$.

($A4$) Any edges connecting $a_i$ with $b_j$, $b_i$ with $c_j$, or $c_i$ with $a_j$ $(i \neq j)$ of weight $w$ in $G$ will contribute weight $w$ in each direction to the edge connecting the vertices $(a_i, b_i, c_i)$ and $(a_j, b_j, c_j)$ in $G_a$.

The adjacency matrix of $G_a$ corresponds to the submatrix $A_a$ in the matrix reduction procedure outlined above. Furthermore, the process leading to $G_a$ from $G$ with a three-fold symmetry element is completely analogous to the process leading to $G_g$ from $G$ with a two-fold symmetry element discussed above.

The two identical components $G_e$ of the disconnected graph $G^*$ each have $q$ vertices corresponding to the identified triplets $(a_1, b_1, c_1), \ldots, (a_q, b_q, c_q)$. The $p$ vertices corresponding to $z_1, \ldots, z_p$ in $G$ vanish in $G_e$. The edges in $G_e$ arise from those of $G$ as follows:

($E1$) Edges of the following types in $G$ involving the vertices $z_i$ all vanish completely in $G_e$:

a) Edges connecting $z_i$ and $z_j$ in $G$;

b) Edges connecting $z_i$ with $a_j$, $b_j$, and $c_j$ in $G$.

(*E*2) Edges connecting $a_i$ and $a_j$ in $G$ of weight $w$ will contribute weight $w$ in each direction to the edge between $(a_i, b_i, c_i)$ and $(a_j, b_j, c_j)$ in $G_e$.

(*E*3) The three edges of a triangle $a_ib_ic_i$ of weight $w$ in $G$ will appear as a loop of weight $-w$ attached to the vertex $(a_i, b_i, c_i)$ in $G_e$.

(*E*4) Any edges connecting $a_i$ with $b_j$, $b_i$ with $c_j$, or $c_i$ with $a_j$ $(i \neq j)$ of weight $w$ in $G$ will contribute weight $-w$ in each direction to the edge connecting the vertices $(a_i, b_i, c_i)$ and $(a_j, b_j, c_j)$ in $G_e$.

Existence of edges of $G$ of both type $E2$ and type $E4$ of weight $w$ between two orbits $a_ib_ic_i$ and $a_jb_jc_j$ of $G$ such as those found in a trigonal antiprism will lead to an edge with weight $-w$ in each direction between the identified vertices $(a_i, b_i, c_i)$ and $(a_j, b_j, c_j)$ in $G_e$. The adjacency matrix of $G_e$ corresponds to the submatrix $A_e$ in the matrix reduction procedure outlined above.

The combined eigenvalues of the three components of the disconnected graph $G^*$ (i.e. $G_a$ and two identical components $G_e$) as defined above will be the eigenvalues of the original connected graph $G$ since this graph splitting process corresponds to the matrix reduction process outlined above. Thus the graphs $G_a$ and $G_e$ have the adjacency matrices $A_a$ and $A_e$, respectively; the combined eigenvalues of $A_a$, $A_e$, and $A_e$ are the same as those of $A''$; and the eigenvalues of $A''$ are the same as those of $A$, the adjacency matrix of $G$. Since two of the components of $G^*$ (i.e. $G_e$) are identical, the eigenvalues of $G$ arising from $G_e$ will have a multiplicity of at least 2.

If the graph to be split contains several two- and/or three-fold symmetry elements, the graph splitting algorithm given above can be repeated several times using the different symmetry elements to achieve maximum splitting to a disconnected graph $G^{**}$ with the maximum number of components. This minimizes the numbers of vertices in any individual components. This simplifies the calculation of the characteristic polynomials of each component by minimizing the numbers of vertices of the sesquivalent edge-subgraphs that have to be considered [1, 12]. Furthermore, the maximum degree of the equations which must be solved to obtain the eigenvalues of each individual component is minimized. If the symmetry elements of $G$ are sufficient, it is useful to reduce $G$ into a disconnected graph $G^{**}$ with individual components containing no more than two vertices apiece. The characteristic polynomials of each component are then very simple to calculate and the resulting quadratic equations are very simple to solve by standard methods. In any case, after all of the two- and three-fold symmetry elements of the original graph $G$ have been used for successive applications of the graph splitting algorithms as outlined above, the characteristic polynomials for each component of the completely split graph $G^{**}$ can be computed by standard methods [1, 12] using the number of sesquivalent edge-subgraphs in each component to determine the coefficients of the corresponding characteristic polynomial. The extensions of these standard procedures of determining characteristic polynomials to the digraphs $G^{**}$ arising from the graph splitting algorithm which inevitably have non-unit and sometimes even negative edge weights as well as different weights of a given edge in opposite directions are trivial as well as apparent from the actual examples to follow.

## 4. Examples of the Graph Splitting Algorithm

### *4.1. The Square Antiprism (Fig. 1)*

The square antiprism is an example of a graph where repeated application of the

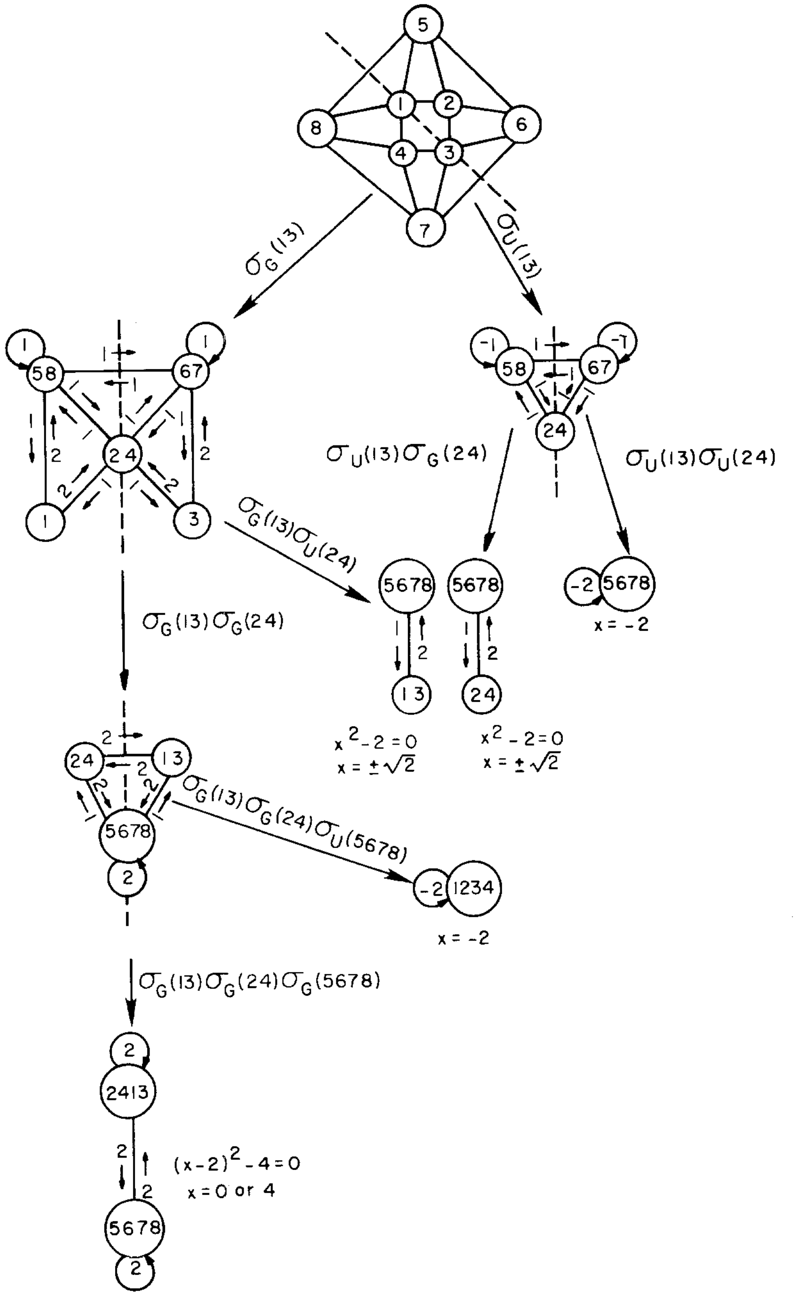


Fig. 1. Application of the graph splitting algorithm to the square antiprism

graph splitting algorithm using the different reflection planes for two-fold symmetry elements as depicted in Fig. 1 results in splitting into a disconnected graph with five components with only one or two vertices apiece and with eigenvalues corresponding to the eigenvalues of the original square antiprism. Determination of the eigenvalues of the square antiprism thus requires the calculation of characteristic polynomials of graphs with no more than two vertices and the solution of only very simple linear and quadratic equations.

### *4.2. The 3,3-Bicapped Trigonal Prism (Fig. 2)*

The 3,3-bicapped trigonal prism is an example of a graph where it is advantageous to start with the three-fold axis in applying the graph splitting algorithm. The first step in the graph splitting algorithm leads to immediate splitting of the original connected graph with eight vertices into a disconnected graph with one component containing four vertices obtained through process $C_{3A}$ (18) and two identical components each containing two vertices each obtained through process $C_{3E}$(18). The four vertex component can be split further by a second application of the graph splitting algorithm using the reflection plane.

### *4.3. Other Graphs Corresponding to Polyhedra with Nine or Less Vertices (Table 1 and Fig. 3)*

Table 1 summarizes further examples of applications of the graph splitting algorithm to graphs corresponding to polyhedra with nine or less vertices as depicted in Fig. 3, which gives details of the vertex numbering schemes used for each polyhedron. Each graph is classified according to the numbers of vertices ($v$), edges ($e$), and faces ($f$) of the corresponding polyhedron. The symmetry properties of each polyhedron are classified by the symmetry point group (Schoenflies notation [11]) and the number of orbits corresponding to the vertices and edges. Further properties of these polyhedra are described in more detail in other papers [2-6].

Possible and effective symmetry element sequences for application of the graph splitting algorithm to the polyhedra in Table 1 are listed there according to the following conventions:

a) The symbols $\sigma$, $C_2$, and $C_3$ refer to reflection planes, two-fold rotation axes, and three-fold rotation axes, respectively.
b) The vertices remaining fixed under a particular symmetry operation ($\sigma$, $C_2$, or $C_3$) are listed in the set of parentheses to the right of the corresponding symmetry element designation using the vertex numbering schemes in Fig. 3. If no numbers appear in parentheses after a particular symmetry element, then no vertices remain fixed under the corresponding symmetry operation.
c) The sequence of using the symmetry elements is from left to right.

From Table 1 and Fig. 3 it is possible to derive figures representing application of the graph splitting algorithm similar to Figs. 1 and 2 for the square antiprism and 3,3-bicapped trigonal prism, respectively.

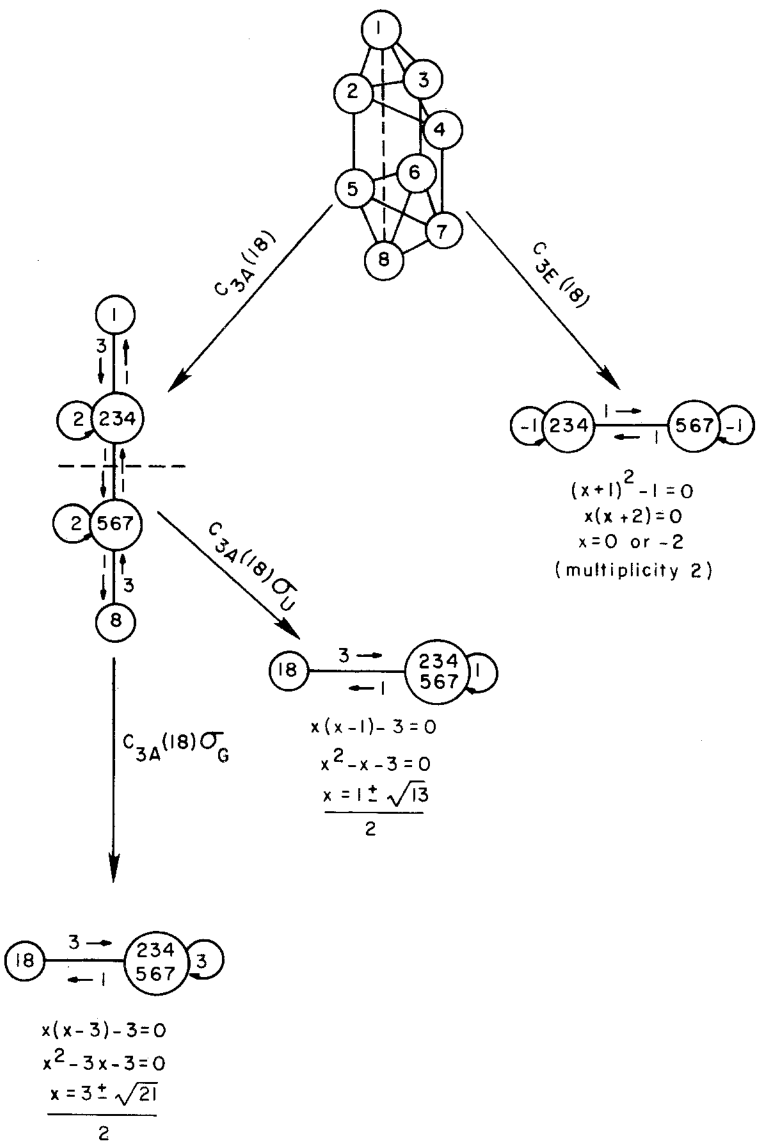


Fig. 2. Application of the graph splitting algorithm to the 3,3-bicapped trigonal prism illustrating the use of a three-fold rotation axis

The results of the graph splitting algorithm can be checked by using the relationships $\Sigma_{i=1}^{v} \lambda_i = 0$ and $\Sigma_{i=1}^{v} \lambda_i^2 = 2e$ [1] where $\lambda_i$ $(i = 1, \ldots, v)$ represents the eigenvalues obtained by solving the factored characteristic polynomial in descending order provided that an eigenvalue of non-unit multiplicity $m$ is counted $m$ times (i.e. $\lambda_j = \lambda_{j+1} = \ldots = \lambda_{j+m-1}$ in the above relationships). The relationship $\Sigma_{i=1}^{v} \lambda_j^3 = 6c_3$ also appears to hold where $c_3$ is the number of circuits of the graph with length 3. In using this last relationship it must be recognized that not all circuits of a graph of

Table 1. Examples of applications of the graph reduction algorithm to the graphs of some polyhedra with nine or less vertices

| Polyhedron Number | v | e | f | Point Group | Factoring Sequence | Characteristic Polynomial | Vertex Orbits | Edge Orbits |
|---|---|---|---|---|---|---|---|---|
| Four and Five Vertex Polyhedra | | | | | | | | |
| 1 (Tetrahedron) | 4 | 6 | 4 | $T_d$ | $\sigma(23)\sigma(14)$ or $C_3(1)$ | $(x-3)(x+1)^3$ | 1 | 1 |
| 2 (Square Pyramid) | 5 | 8 | 5 | $C_{4v}$ | $\sigma(124)\sigma(135)\sigma(1)$ | $x^2(x+2)(x^2-2x-4)$ | 2 | 2 |
| 3 (Trigonal Bipyramid) | 5 | 9 | 6 | $D_{3h}$ | $\sigma(234)\sigma(135)$ or $C_3(15)\sigma(234)$ | $x(x+1)^2(x^2-2x-6)$ | 2 | 2 |
| Six Vertex Polyhedra | | | | | | | | |
| 4 (Trigonal Prism) | 6 | 9 | 5 | $D_{3h}$ | $\sigma\sigma(14)$ or $C_3\sigma$ | $x^2(x-3)(x-1)(x+2)^2$ | 1 | 2 |
| 5 (Pentagonal Pyramid) | 6 | 10 | 6 | $C_{5v}$ | $\sigma(15)$ | $(x^2+x-1)^2(x^2-2x-5)$ | 2 | 2 |
| 6 | 6 | 11 | 7 | $C_{2v}$ | $\sigma(1246)\sigma(35)$ | $x(x^2+x-1)(x^3-x^2-9x-4)$ | 3 | 4 |
| 7 (Octahedron) | 6 | 12 | 8 | $O_h$ | $\sigma(2345)\sigma(1246)\sigma(1356)\sigma(24)$ | $x^3(x-4)(x+2)^2$ | 1 | 1 |
| Seven Vertex Polyhedra | | | | | | | | |
| 8 | 7 | 11 | 6 | $C_{2v}$ | $\sigma(1)\sigma(167)$ | $(x-1)(x+1)(x^2+2x-1)(x^3-2x^2-5x+4)$ | 3 | 4 |
| 9 (3-Capped Trigonal Prism) | 7 | 12 | 7 | $C_{3v}$ | $C_3(1)$ | $x^2(x+2)^2(x^3-4x^2+6)$ | 3 | 4 |
| 10 (Hexagonal Pyramid) | 7 | 12 | 7 | $C_{6v}$ | $C_3(1)\sigma(1)$ | $(x-1)^2(x+1)^2(x+2)(x^2-2x-6)$ | 2 | 2 |
| 11 (4-Capped Trigonal Prism) | 7 | 13 | 8 | $C_{2v}$ | $\sigma(1)\sigma(167)$ | $x(x-1)(x+2)^2(x^3-3x^2-4x+4)$ | 3 | 4 |
| 12 | 7 | 14 | 9 | $C_{2v}$ | $\sigma(23456)\sigma(147)$ | $x(x-1)(x+1)(x^4-13x^2-16x+2)$ | 4 | 5 |
| 13 (Pentagonal Bipyramid) | 7 | 15 | 10 | $D_{5h}$ | $\sigma(23456)\sigma(137)$ | $x(x^2+x-1)^2(x^2-2x-10)$ | 2 | 2 |
| 14 (Capped Octahedron) | 7 | 15 | 10 | $C_{3v}$ | $C_3(1)$ | $x^2(x+2)^2(x^3-4x^2-3x+6)$ | 3 | 4 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Eight Vertex Polyhedra | | | | | | | | | |
| 15 | (Cube) | 8 | 12 | 6 | $O_h$ | $\sigma\sigma'$ | $(x-3)(x-1)^3(x+1)^3(x+3)$ | 1 | 1 |
| 16 | | 8 | 13 | 7 | $C_{2v}$ | $\sigma(1357)\sigma(2468)$ | $(x-1)(x+1)(x^2+x-1)(x^4-x^3-10x^2+5x+9)$ | 4 | 4 |
| 17 | | 8 | 14 | 8 | $D_{2h}$ | $\sigma\sigma(3456)\sigma(1278)$ | $x(x-1)(x+1)(x+2)(x^2-3x-2)(x^2+x-4)$ | 2 | 3 |
| 18 | (3,3-Bicapped Trigonal Prism) | 8 | 15 | 9 | $D_{3h}$ | $\sigma\sigma(1836)\sigma(4725)$ or $C_3(18)\sigma$ | $x^2(x+2)^2(x^2-3x-3)(x^2-x-3)$ | 2 | 3 |
| 19 | (Square Antiprism) | 8 | 16 | 10 | $D_{4d}$ | $\sigma(13)\sigma(24)\sigma(5678)$ | $x(x-4)(x+2)^2(x^2-2)^2$ | 1 | 2 |
| 20 | (4,4-Bicapped Trigonal Prism) | 8 | 17 | 11 | $C_{2v}$ | $\sigma(78)\sigma(14)$ | $(x-1)(x+2)^2(x^2-2)(x^3-3x^2-6x+2)$ | 3 | 5 |
| 21 | | 8 | 18 | 12 | $D_{2d}$ | $\sigma(3478)\sigma(1256)C_2$ | $(x^2-3x-7)(x^2+x-3)(x^2+x-1)^2$ | 2 | 4 |
| 22 | (Bicapped Octahedron) | 8 | 18 | 12 | $D_{3d}$ | $C_3(18)\sigma$ | $x(x+2)(x^2-3)(x^2-4x-3)$ | 2 | 3 |
| 23 | (Hexagonal Bipyramid) | 8 | 18 | 12 | $D_{6h}$ | $C_3(18)\sigma(18)\sigma(234567)$ | $(x-1)^2(x+1)^2x(x+2)(x^2-2x-12)$ | 2 | 2 |
| Nine Vertex Polyhedra | | | | | | | | | |
| 24 | | 9 | 15 | 8 | $D_{3h}$ | $C_3\sigma(456)$ | $(x-2)(x+1)^2(x^2-4x+2)(x^2+2x-1)^2$ | 2 | 3 |
| 25 | (Capped Cube) | 9 | 16 | 9 | $C_{4v}$ | $\sigma(12478)\sigma(13579)\sigma$ | $(x-1)^2(x+1)^3(x+3)(x^3-4x^2-x+8)$ | 3 | 4 |
| 26 | | 9 | 17 | 10 | $C_{2v}$ | | | | |
| 27 | | 9 | 18 | 11 | $D_{3h}$ | $C_3\sigma(456)$ | $(x-4)(x-2)(x-1)^2(x+1)^2(x+2)^3$ | 2 | 2 |
| 28 | | 9 | 19 | 12 | $C_{2v}$ | | | | |
| 29 | (4-Capped Square Antiprism) | 9 | 20 | 13 | $C_{4v}$ | $\sigma(135)\sigma(124)\sigma(16789)$ | $(x+2)^2(x^2-2)^2(x^3-4x^2-4x+8)$ | 3 | 4 |
| 30 | (4,4,4-Tricapped Trigonal Prism) | 9 | 21 | 14 | $D_{3h}$ | $C_3\sigma(456)$ | $(x-1)(x+2)^2(x^2-2)^2(x^2-3x-8)$ | 2 | 3 |

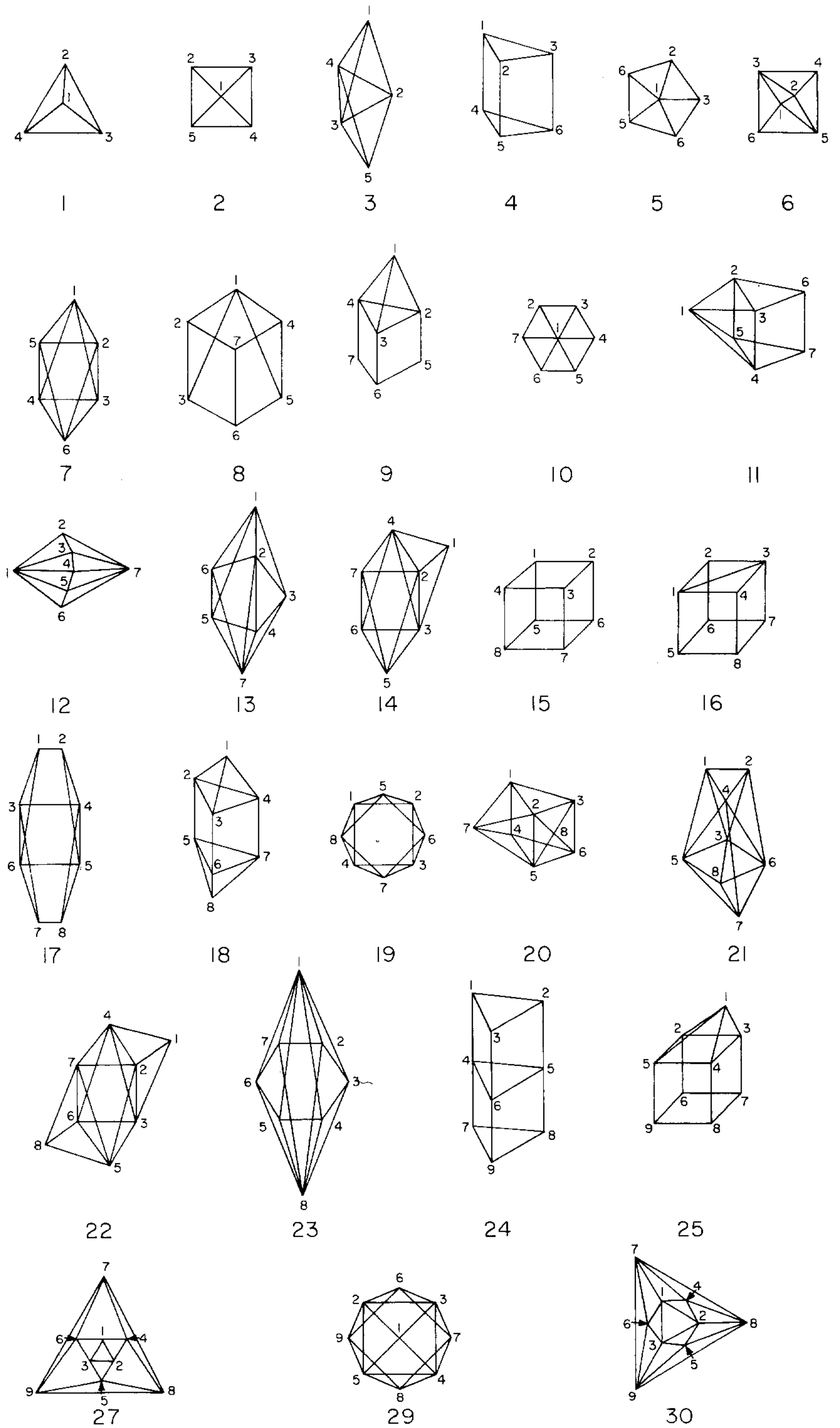


Fig. 3. The polyhedra in Table 1 and the numbering scheme for their vertices

length 3 may correspond to triangular faces of the corresponding polyhedron. For example, the trigonal bipyramid (polyhedron 3 in Fig. 3) has six triangular faces but the corresponding graph has seven circuits of length 3. The "extra" circuit of length 3 in the graph of the trigonal bipyramid which does not correspond to a polyhedral face is the one connecting the equatorial vertices (2, 3, and 4 in Fig. 3). Similar relations of the type $\Sigma_{i=1}^{v} \lambda_i^n = xy$ ($x$ = integer, $y$ = the number of some type of circuit, etc.) for $n > 3$ are more complex and less useful since, for example, both the circuit graph $C_4$ (quadrilateral) and the four-vertex graph having two disjoint edges are sesquivalent graphs with four vertices.

## 5. Eigenvalues of Some Generalized Families of Polyhedra with Two Edge Orbits

All of the previous calculations of the characteristic polynomials of graphs corresponding to polyhedra assume that all edges of the original polyhedron, and therefore of the corresponding graph, are of unit weight even if they are in different orbits where equal edge weights are not demanded by the symmetry properties. This section considers a different type of eigenvalue calculation of families of polyhedra with two edge orbits where the relative weights of the edges in the two different edge orbits are continuously varied. Such calculations are potentially useful in chemical problems for evaluating the effects of distortions of an array of atoms on the energy levels of the system.

The families of polyhedra with two edge orbits considered here are the prisms, pyramids, and bipyramids. In each of these families one type of edge connects vertices to form polygons corresponding to the highest order rotation axis. This first type of edge will be given unit weight. The second type of edge either connects the corresponding vertices of two identical polygons in the case of the prisms or the vertices of a polygon to one or two external points in the cases of the pyramids and bipyramids, respectively. This second type of edge will be given weight $w$. This method of designating the edge weights of polyhedra with two edge orbits provides information on the completely general case, since if the edges of the polyhedron of the first type do not have unit weight but instead weight $x$ ($x \neq 1$) and the edges of the second type have weight $y$, then set $w = y/x$ and multiply the resulting eigenvalues by $x$.

### *5.1. Prisms*

A prism $T_n$ consists of two identical and parallel polygons $C_n$ with additional edges connecting corresponding vertices in each polygon. Each vertex is of valency 3. There are a total of $3n$ edges in the following two edge orbits: 1) $2n$ equivalent intrapolygonal edges within each $C_n$ polygon; 2) $n$ equivalent interpolygonal edges connecting equivalent vertices of each polygon. Give the $2n$ intrapolygonal edges weight 1 and the $n$ interpolygonal edges weight $w$. Then the adjacency matrix of $T_n$ has the form

$$\begin{pmatrix} C_n & wI_n \\ wI_n & C_n \end{pmatrix}$$

where $C_n$ is the adjacency matrix of the polygon $C_n$ and $I_n$ is the $n \times n$ matrix with +1's on the diagonal and zeroes elsewhere. Reduce this matrix through the reflection plane of the prism which bisects the interpolygonal edges using the procedure outlined earlier in this paper noting that corresponding vertices of the two equivalent $C_n$ polygons are in the same orbit under this reflection plane. This matrix reduction proceeds as follows:

$$A' = \begin{pmatrix} C_n + wI_n & wI_n \\ C_n + wI_n & C_n \end{pmatrix} \qquad A'' = \begin{pmatrix} C_n + wI_n & wI_n \\ 0 & C_n - wI_n \end{pmatrix}$$

The eigenvalues of the resulting matrix $A''$ are $E(C_n) + w$ and $E(C_n) - w$ where $E(C_n)$ are the eigenvalues of the adjacency matrix of $C_n$. In other words the eigenvalues of a prism are obtained by subtracting and adding the weight of the interpolygonal edges to the eigenvalues of the identical and parallel $C_n$ polygons forming the upper and lower faces.

### 5.2. *Standard Reduction of the Adjacency Matrix $C_n$*

Before considering the eigenvalues of pyramids and bipyramids it is first necessary to develop a standard reduction of the adjacency matrix of a regular polygon $C_n$ with $n$ sides. This procedure uses the symmetry of the $n$-fold rotation axis of $C_n$ to reduce its adjacency matrix $C_n$ by the following two-step process corresponding completely to the matrix reduction procedure outlined earlier in this paper.

a) Add columns $2, 3, \ldots, n$ to column 1. This will give each entry in column 1 the value +2 since each vertex in a regular polygon is connected to exactly two other vertices.
b) Subtract row 1 from each of the rows $2, 3, \ldots, n$ to give a matrix $M_n$ of the form

$$\begin{pmatrix} 2 & \text{immaterial} \\ 0 & U_n \end{pmatrix}.$$

The first step above consists of right multiplying $C_n$ by a unit lower triangular matrix $P$ with +1's on the main diagonal, +1's in the first column, and zeroes elsewhere. The second step above consists of left multiplication by another unit lower triangular matrix $Q$ with +1's on the main diagonal, −1's in the non-diagonal first column positions, and zeroes elsewhere. As in the case of the adjacency matrix reduction procedure for graphs with two- and three-fold symmetry elements discussed earlier in this paper, $PQ = I$ and therefore $Q = P^{-1}$. The two-step procedure given above is therefore a similarity transformation and the eigenvalues of $M_n$ are thus the same as those of $C_n$. The eigenvalues of $U_n$ designated as $E(U_n)$ are the same as those of $C_n$ except for deletion of +2.

This generalized method for reducing the adjacency matrix $C_n$ will be used when studying the eigenvalues of pyramids and bipyramids and will be called the standard reduction of $C_n$.

### 5.3. *Pyramids*

A pyramid $W_n$ (also known as a wheel) is the cone [1] of a regular polygon $C_n$ where each vertex of the polygon $C_n$ is connected by an additional edge to an external point called the apex. The polygonal vertices each have valency 3 whereas the apex has valency $n$. The pyramid $W_n$ has a total of $2n$ edges in the following two edge orbits: 1) $n$ equivalent intrapolygonal edges within the basal polygon; 2) $n$ equivalent apical edges connecting the apex with each vertex of the basal polygon. Give the $n$ intrapolygonal edges weight 1 and the $n$ apical edges weight $w$. The adjacency matrix of $W_n$ has the following general form if the first row and column correspond to the apex and if $j_n$ is the $1 \times n$ column vector or the $n \times 1$ row vector with all entries +1:

$$\begin{pmatrix} 0 & wj_n \\ wj_n & C_n \end{pmatrix}.$$

Apply the standard reduction discussed above to $C_n$ except during the second step include the first column corresponding to the apex in the usual row subtraction process. This gives

$$\begin{pmatrix} 0 & nw & ? \\ w & 2 & ? \\ 0 & 0 & U_n \end{pmatrix}$$

where the ? entries are immaterial. Note that this matrix factors into a $2 \times 2$ matrix and the matrix $U_n$ identical to that obtained in the standard reduction of $C_n$ discussed above.

The eigenvalues of the $2 \times 2$ matrix are $1 \pm \sqrt{1 + nw^2}$ whereas the eigenvalues of $U_n$ are those of $C_n$ with deletion of +2. Thus the addition of an apex to a polygon $C_n$ to form the corresponding pyramid $W_n$ splits the +2 eigenvalue of $C_n$ into two eigenvalues centered at +1 with their separation increasing with increasing weight of the apical edges but leaves unaffected the remaining eigenvalues of the polygon $C_n$.

### 5.4. *Bipyramids*

A bipyramid $\Pi_n$ is the suspension of a regular polygon $C_n$ where each vertex of the equatorial polygon $C_n$ is connected by additional edges to each of two external points called the apices. The polygonal vertices have valency 4 whereas the apices have valency $n$. There are a total of $3n$ edges in the following two-edge orbits: 1) $n$ equivalent intrapolygonal edges within the equatorial polygon; 2) $2n$ equivalent apical edges connecting each apex with each vertex of the equatorial polygon. Give the $n$ intrapolygonal edges weight 1 and the $2n$ apical edges weight $w$. The adjacency matrix of $\Pi_n$ has the following form if the two last rows and columns correspond to the apices:

$$\begin{pmatrix} C_n & wj_n & wj_n \\ wj_n & 0 & 0 \\ wj_n & 0 & 0 \end{pmatrix}.$$

Reduce this matrix through the reflection plane containing all of the vertices of the equatorial polygon using the procedure outlined earlier in this paper. This reduction proceeds as follows:

$$A' = \begin{pmatrix} C_n & 2wj_n & wj_n \\ wj_n & 0 & 0 \\ wj_n & 0 & 0 \end{pmatrix} \quad A'' = \begin{pmatrix} C_n & 2wj_n & wj_n \\ wj_n & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The eigenvalues are therefore 0 and the $n + 1$ eigenvalues of an $(n + 1) \times (n + 1)$ matrix which will be reduced further.

Before proceeding with this further reduction of $A''$ relabel and rearrange the rows and columns of this $(n + 1) \times (n + 1)$ matrix to make the last row and column (arising from the apices) the first row and column giving

$$\begin{pmatrix} 0 & wj_n \\ 2wj_n & C_n \end{pmatrix}.$$

Note that this process preserves the diagonal elements.

Next apply the standard reduction to $C_n$ discussed above except during the second step include in the subtraction process the first column originating from the apices. This gives

$$\begin{pmatrix} 0 & nw & ? \\ 2w & 2 & ? \\ 0 & 0 & U_n \end{pmatrix}$$

where the ? entries are immaterial. Note that this matrix factors into a $2 \times 2$ matrix and the matrix $U_n$ identical to that obtained in the standard factoring of $C_n$ discussed above. The eigenvalues of the $2 \times 2$ matrix are $1 \pm \sqrt{1 + 2\,nw^2}$ whereas the eigenvalues of $U_n$ are those of $C_n$ with deletion of +2. Thus the addition of two apices to a regular polygon $C_n$ to form the corresponding bipyramid leads to a new zero eigenvalue and splits the +2 eigenvalue into two eigenvalues centered at +1 but leaves unaffected the remaining eigenvalues of the basal polygon.

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