

Computer Perception of Molecular Symmetry

K. Balasubramanian

Department of Chemistry and Biochemistry, Arizona State University, Tempe, Arizona 85287-1604

Received March 21, 1995*

A computer code and algorithm are developed for the computer perception of molecular symmetry. The code generates and uses the Euclidian distance matrices of molecular structures to generate the permutation-inversion group of the molecule. The permutation-inversion group is constructed as the automorphism group of the Euclidian distance matrix. Applications to several molecular structures and fullerenes such as the C₆₀ buckminsterfullerene and C₂₈ and C₂₄ fullerenes are considered.

1. INTRODUCTION

An important and fundamental question in chemical applications of artificial intelligence pertains to the development of algorithms for the machine perception of molecular symmetry. One of the difficulties with the machine perception of molecular symmetry is that the conventional human perception of the molecular symmetry that involves pattern recognition cannot be easily transferred as an algorithm to a computer. That is, the machine learning techniques and algorithms for the machine perception of symmetry can be complex. Often the information stored for a molecule in the computer is in the form of internal or Cartesian coordinates or in the form of a set of bond lengths, bond angles, and dihedral angles. The last representation would require a neural network for computer representation of a structure. A difficulty associated with the Cartesian coordinates is that they depend on the coordinate axis and are not invariant to operations such as rotations, reflections, and translations.

Perhaps a major source of difficulty is in the machine perception of the highest-fold rotational axis of a molecule purely from the Cartesian coordinates as the coordinates depend on the frame of reference. However, for specific cases this could be overcome by appropriately embedding the molecule such that the geometrical center coincides with the origin of the reference frame.

In the current investigation we develop very general algorithms that yield the molecular symmetry from structurally-invariant matrices called the Euclidian distance matrices. That is, the Euclidian distances in the matrices associated with molecules are invariant to rotations, reflections, inversion, improper rotations, translations, etc., and are chosen as structural invariants. The Euclidian distances between the various nuclei in the molecule are shown to offer novel matrix representation of the geometric and structural features of a molecule. It is shown that the permutations of the nuclei that leave the Euclidian matrix of the molecule invariant comprise the permutations contained in the permutation-inversion group of a molecule defined by Longuet-Higgins in 1963.¹ The automorphism group of the Euclidian matrix is constructed by the algorithm and the code developed here.

Computational techniques for the automorphism groups of graphs have been the topic of several investigations.²⁻¹¹ The Euclidian matrix representation which encompasses the

stereochemistry of a molecule¹¹⁻¹⁵ as well as the conformation of a rigid molecular structure can indeed be envisaged as a weighted graph, and, consequently, the automorphism group of the associated weighted graph can be sought for the machine perception of the associated molecular symmetry. In recent years several investigators¹¹⁻¹⁵ have used the Euclidian distance matrices for developing three-dimensional molecular structural descriptors. Indeed the graph theoretical techniques provided the motivation for the algorithms described in the current investigation.

The algorithm and code developed here are applied to several molecules in their rigid conformations as well as fullerenes such as the C₆₀ buckminsterfullerene and C₂₈ and C₂₄ fullerenes. Fullerenes are topical species, and it is thus interesting that the techniques developed here can be applied to fullerenes. Unlike other approaches which at best perceive the molecular symmetry as a point group, it is shown that the technique developed here yields directly the permutation-inversion group. The permutation-inversion group plays an important role in the structure and spectroscopy of molecules.^{2,17-19} Furthermore all other groups such as the edge group, face group, ring group, frame group, etc., associated with molecules can be easily obtained from the permutation inversion group in conjunction with the Euclidian and other matrices. Moreover, nuclear spin statistics of the rovibronic levels, nuclear spin functions, the hyperfine patterns in ESR, etc., could be obtained readily from the permutation-inversion group. The symmetry-adapted linear combination¹⁹ (SALC) of atomic orbitals of large polyatomic systems could also be generated from the permutation-inversion groups.

2. COMPUTATIONAL TECHNIQUES FOR THE MACHINE PERCEPTION OF MOLECULAR SYMMETRY

A. Euclidian Matrices and Their Automorphism Groups. The three-dimensional Euclidian distance between two nuclei is defined as

$$d_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$$

where (x_i, y_i, z_i) and (x_j, y_j, z_j) are the coordinates of the nuclei i and j , respectively. The Euclidian distance matrix of a

* Abstract published in *Advance ACS Abstracts*, May 15, 1995.

molecule is defined as

$$D_{ij} = \begin{cases} d_{ij} & \text{if } i \neq j \text{ where } d_{ij} \text{ is the Euclidian distance} \\ & \text{between the nuclei } i \text{ and } j \\ 0 & \text{if } i = j \end{cases}$$

The Euclidian distance matrix thus defined does not depend on the coordinate axis and is thus invariant to rotational, transitional, and reflection operations, whereas the internal coordinates such as bond lengths, bond angles, and dihedral angles depend on the atoms that are used to define them. The Euclidian matrix provides a direct matrix representation that can be used for matrix manipulations, eigenvector computations, etc.

A permutation of the nuclei in the molecule is an automorphic permutation, if it preserves the Euclidian distances. In formal terms this can be defined if we introduce the permutation matrices for permutations. A permutation of the nuclei of the molecule can be described by the permutation matrix **P** defined as

$$P_{ij} = \begin{cases} 1 & \text{if the nucleus } i \text{ is permuted to the nucleus } j \\ 0 & \text{otherwise} \end{cases}$$

A permutation is in the automorphism group of the Euclidian matrix if the permutation matrix **P** satisfies

$$P^T D P = D$$

where **P**^T is the transpose of the permutation matrix. Such a permutation would also represent a proper or improper rotation of the molecule. All such permutations of the nuclei that preserve the Euclidian distance matrix of the molecular structure form a group which was called the Euclidian distance group by the author.¹¹ The current author¹¹ showed that the Euclidian distance group is isomorphic to the permutation-inversion group of Longuet-Higgins¹ if the improper rotations in the point group generate new permutations not already contained in the permutational representation of proper rotational operations. If the improper rotational operations such as the mirror planes, inversion operations, etc., generate the same permutations as the ones obtained by proper rotational subgroup, then the Euclidian distance group is shown to contain only the unique permutations thus containing only half the number of elements in the point group of the molecule.

The Euclidian distance group can be illustrated with the ethane molecule in an eclipsed conformation. For the purpose of symmetry perception, it suffices to set all C-H and C-C bond lengths to units in the ethane molecule and consider only the Euclidian distances between the various hydrogen atoms in the molecule. The Euclidian distance matrix of the eclipsed ethane molecule in terms of these distances for the hydrogen nuclei is given by

$$D = \begin{bmatrix} 0 & \sqrt{3} & \sqrt{3} & 1 & 2 & 2 \\ \sqrt{3} & 0 & \sqrt{3} & 2 & 1 & 2 \\ \sqrt{3} & \sqrt{3} & 0 & 2 & 2 & 1 \\ 1 & 2 & 2 & 0 & \sqrt{3} & \sqrt{3} \\ 2 & 1 & 2 & \sqrt{3} & 0 & \sqrt{3} \\ 2 & 2 & 1 & \sqrt{3} & \sqrt{3} & 0 \end{bmatrix}$$

A permutation is an automorphic permutation if it preserves

the above Euclidian matrix. For example, the permutation (1 6 2 4 3 5) of the nuclei is an automorphic permutation. The permutation matrix associated with this permutation is given by

$$P = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The result of multiplying **P**^T on the left and **P** to the right of the Euclidian distance matrix is shown below:

$$P^T D P = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & \sqrt{3} & \sqrt{3} & 1 & 2 & 2 \\ \sqrt{3} & 0 & \sqrt{3} & 2 & 1 & 2 \\ \sqrt{3} & \sqrt{3} & 0 & 2 & 2 & 1 \\ 1 & 2 & 2 & 0 & \sqrt{3} & \sqrt{3} \\ 2 & 1 & 2 & \sqrt{3} & 0 & \sqrt{3} \\ 2 & 2 & 1 & \sqrt{3} & \sqrt{3} & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 2 & 2 & 1 & \sqrt{3} & \sqrt{3} & 0 \\ 1 & 2 & 2 & 0 & \sqrt{3} & \sqrt{3} \\ 2 & 1 & 2 & \sqrt{3} & 0 & \sqrt{3} \\ \sqrt{3} & \sqrt{3} & 0 & 2 & 2 & 1 \\ 0 & \sqrt{3} & \sqrt{3} & 1 & 2 & 2 \\ \sqrt{3} & 0 & \sqrt{3} & 2 & 1 & 2 \end{bmatrix} = \begin{bmatrix} 0 & \sqrt{3} & \sqrt{3} & 1 & 2 & 2 \\ \sqrt{3} & 0 & \sqrt{3} & 2 & 1 & 2 \\ \sqrt{3} & \sqrt{3} & 0 & 2 & 2 & 1 \\ 1 & 2 & 2 & 0 & \sqrt{3} & \sqrt{3} \\ 2 & 1 & 2 & \sqrt{3} & 0 & \sqrt{3} \\ 2 & 2 & 1 & \sqrt{3} & \sqrt{3} & 0 \end{bmatrix}$$

Consequently, multiplying the transpose of the permutation matrix on the left side and the permutation matrix itself to the right yields the Euclidian matrix that we started with, and, consequently, the permutation (1 6 2 4 3 5) preserves the Euclidian distance matrix of the eclipsed conformation of ethane. Thus this permutation belongs to the automorphism group of the Euclidian distance matrix.

The above exercise can be repeated for the permutation (1 2 3 4 5 6), and it can be shown that the result that the result of multiplying **P**^T on the left and **P** on the right side yields a new matrix that is different from the original Euclidian distance matrix that we start with for the ethane molecule in the eclipsed conformation. Thus the permutation

(1 2 3 4 5 6) does not belong to the automorphism group of the rigid ethane molecule in the eclipsed conformation.

If one collects all of the permutations of the nuclei that preserve the Euclidian distance matrix into a set, the set would form a group called the Euclidian distance group. The Euclidian distance group of the eclipsed conformation of ethane is thus given by

$$G = \{(1)(2)(3)(4)(5)(6), (1\ 2)(3)(4\ 5)(6), \\ (1\ 6)(2\ 5)(3\ 4), (1\ 6\ 2\ 4\ 3\ 5), \\ (1\ 4)(2\ 6)(3\ 5), (1\ 5\ 3\ 4\ 2\ 6), (1\ 5)(2\ 4)(3\ 6), \\ (1\ 4)(2\ 5)(3\ 6), (1\ 3\ 2)(4\ 6\ 5), (1\ 3)(2)(4\ 6)(5), \\ (1\ 2\ 3)(4\ 5\ 6), (1)(2\ 3)(4)(5\ 6)\}$$

We use the standard orbit notation for denoting the permutation. For example, the notation (1 2 3 ... *i*) means 1 goes to 2, 2 goes to 3, ..., and finally *i* goes to the position of the starting vertex, which is 1 in this case. Thus the notation (1 2)(3)(4 5)(6) means 1 goes to 2, 2 goes to 1, 3 goes to itself, 4 goes to 4, 5 goes to 4, and 6 goes to itself. The resulting group of 12 permutations is isomorphic to the D_{3h} point group comprising both proper and improper rotations of the ethane molecule in the eclipsed conformation. Note that both proper and improper rotations are generated as permutation operations since the improper axes of rotations generate new permutation representations that are not already contained in the rotational subgroup of the point group.

Let us consider the staggered conformation of the ethane molecule. If the C-C and C-H distances are taken as unities in some arbitrary scale, then the Euclidian distance matrix is given by

$$D = \begin{bmatrix} 0 & \sqrt{3} & \sqrt{3} & \sqrt{2} & \sqrt{5} & \sqrt{2} \\ \sqrt{3} & 0 & \sqrt{3} & \sqrt{5} & \sqrt{2} & \sqrt{2} \\ \sqrt{3} & \sqrt{3} & 0 & \sqrt{2} & \sqrt{2} & \sqrt{5} \\ \sqrt{2} & \sqrt{5} & \sqrt{2} & 0 & \sqrt{3} & \sqrt{3} \\ \sqrt{5} & \sqrt{2} & \sqrt{2} & \sqrt{3} & 0 & \sqrt{3} \\ \sqrt{2} & \sqrt{2} & \sqrt{5} & \sqrt{3} & \sqrt{3} & 0 \end{bmatrix}$$

Although the Euclidian distance matrix of the staggered conformation is different from that of the eclipsed conformation, the automorphism group of the Euclidian distance matrix of the staggered conformation comes out to be identical to that of the eclipsed conformation. The current author¹¹ showed that under judicious choice of mappings of the Euclidian distances the two matrices can be transformed into each other. This is the reason as to why both the staggered and eclipsed conformations have the same permutation-inversion groups, although the point groups of the two conformations differ as D_{3h} and D_{3d} , respectively.

B. The Graph Automorphism Groups. A graph is simply a collection of vertices with a relation defined between the vertices which leads to a set of edges. The adjacency matrix of a graph which is a fundamental representation of the graph is defined as

$$A_{ij} = \begin{cases} 1 & \text{if the vertices } i \text{ and } j \text{ are connected by an edge} \\ 0 & \text{otherwise} \end{cases}$$

A permutation of the vertices of the graph is said to belong

to the automorphism group or it preserves the adjacency matrix. Mathematically,

$$P^T A P = A$$

All such permutations that satisfy the above automorphism condition belong to a group called the automorphism group. Note that this definition of the automorphism group of a graph is similar to that of the Euclidian distance group, the main difference being in the matrices which define the relation between the nuclei. In the Euclidian distance matrices, actual shortest distances between the nuclei are used while in the case of the adjacency matrix, the adjacency relation between the nuclei is used. The Euclidian distance group and the automorphism group are in general not isomorphic to each other.

Let us illustrate the graph automorphism with the graph of benzene. An adjacency matrix of the benzene graph is given by

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

The permutation (1 2 3 4 5 6) is an automorphic permutation of the benzene graph, but the permutation (1 3 2 4 5 6) is not an automorphic permutation. The permutation matrix of the former permutation is given by

$$P = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Consequently, the effect of this permutation on the adjacency matrix

is described by the matrix multiplications shown below:

$$P^T(1\ 2\ 3\ 4\ 5\ 6)AP(1\ 2\ 3\ 4\ 5\ 6) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} = A$$

Consequently, the permutation (1 2 3 4 5 6) belongs to the automorphism group of the benzene molecule. The above process of matrix multiplications can be repeated for the permutation (1 3 2 4 5 6), and it can be shown that the

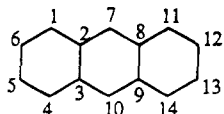


Figure 1. The nuclear labeling for anthracene. See text for the computer perception and equivalence classes.

result of multiplying the permutation matrices does not yield the adjacency matrix back and thus the permutation (1 3 2 4 5 6) does not belong to the automorphism group of the benzene graph.

C. Nuclear Equivalence Classes. Two vertices of a graph are said to be equivalent if there exists an automorphic permutation that transforms one to the other. In the case of benzene graph, all vertices are equivalent since the automorphic permutations transform them to each other. This concept was extended for equivalence classes of nuclei based on Euclidian distance matrices.¹⁶ The algorithm developed by the author for partitioning nuclei into equivalence classes would constitute an appropriate starting point for computer perception of molecular symmetry. For molecules which exhibit more than one nuclear equivalence class, considerable simplification can be achieved through the use of nuclear equivalence classes.

The current author¹⁶ developed a technique based on a multiple-order Euclidian degree algorithm which we briefly describe for the sake of completeness. The Euclidian degree of the nucleus i in the molecule is defined as

$$e_i = \sum_{j \neq i} d_{ij}$$

where d_{ij} 's are Euclidian distances and the sum is over all j except $j = i$. It may be pointed out that the largest Euclidian degree gives the upper bound to the first eigenvalue of the distance matrix. Although the Euclidian degrees may be a starting point, one needs a more rigorous approach. Define the k th order Euclidian degree index as

$$e_i^{(k)} = \frac{1}{s^k} \sum_j D_{ij}^k$$

where D^k is the k th power of the Euclidian distance matrix and s is a scaling factor introduced so that the k th order Euclidian degrees are kept within bounds. The process of computing the equivalence class structures can be iterated starting from the equivalence classes generated with the first order Euclidian degrees. The equivalence classes generated at the current and previous iterations can be compared. If they are the same then convergence is reached and thus the correct nuclear partitioning is generated. If convergence is not reached then the process is iterated until convergence is reached.

Suppose $S_1^{(k)}, S_2^{(k)}, \dots, S_m^{(k)}$ be the disjoint set of nuclear equivalence classes generated in the k th iteration

$$S = S_1^{(k)} \cup S_2^{(k)} \cup \dots \cup S_m^{(k)}$$

$$S_i^{(k)} \cap S_j^{(k)} = \phi$$

where S is the set of nuclei and ϕ is the null set. The algorithm for the k th order Euclidian degree partitions is

```

k ← 1
e_i^1 ← ∑_j d_ij
compute S_1^{(1)} ∪ S_2^{(1)} ∪ ... ∪ S_m^{(1)},
based on {e_1^{(1)}, e_2^{(1)}, ..., e_n^{(1)}}
* k ← k + 1
e_i^k ← ∑_j d_ij^k
compute S_1^{(k)} ∪ S_2^{(k)} ∪ ... ∪ S_m^{(k)}
if m_k · eq · m_{k-1} and
S_j^k · eq · S_j^{(k-1)} then
convergence is reached; exit
else go to *

```

The author¹⁴ investigated the convergence of the k th order Euclidian degree algorithm and found that convergence was reached in two iterations for almost all 50 structures that were tested, and only for one structure third iteration was required. Consequently, the k th order Euclidian degree algorithm is quite efficient and serves the purpose of generating nuclear equivalence classes.

The Euclidian degree algorithm can be illustrated with the anthracene molecule (Figure 1). The first-order Euclidian degrees are given by the set

{33.893 231, 26.643 607, 26.643 607, 33.893 231,
39.608 635, 39.608 635, 27.511 208, 26.643 607,
26.643 607, 27.511 208, 33.893 231,
39.608 635, 39.608 635, 33.893 231}

This results in the following nuclear equivalence classes for anthracene:

{1,4,11,14}, {2,3,8,9}, {5,6,12,13}, {7,10}

The advantages of generating the nuclear equivalence classes are evident. A permutation in the Euclidian distance group can only exchange nuclei in an equivalence class. Two nuclei in different equivalence classes cannot be exchanged by a distance-preserving permutation. This is quite useful in the actual automorphism search.

D. Algorithms for Computer Generation of the Euclidian Distance Group. Let us denote a permutation P in a two-row notation as follows.

$$P = \begin{bmatrix} 1 & 2 & 3 & \dots & i & \dots & n \\ p_1 & p_2 & p_3 & \dots & p_i & \dots & p_n \end{bmatrix}$$

In the above notation the nucleus i gets permuted to the nucleus p_i by the permutation P . The action of the above permutation on the Euclidian distance matrix D can be expressed in terms of the elements p_i 's in the second row without actually performing the matrix multiplications. This results in significant CPU time reduction as shown by the author⁴ in the context of graph automorphisms and the automorphism groups of weighted graphs.³ That is, the ij th matrix element of the permuted Euclidian distance matrix E is related to the original Euclidian matrix D by

$$E_{ij} = D_{p_i p_j}$$

Thus all the matrix elements of the E matrix are contained

in the **D** matrix. There is no need to perform matrix multiplications. This method is more efficient compared to matrix multiplications and leads to the condition that if

$$\mathbf{D}_{p_i p_j} = \mathbf{D}_{ij} \text{ for all } i = 1, n$$

then the permutation **P** belongs to the Euclidian distance group of the molecule.

The algorithm could take advantage of the nuclear equivalence class information. Suppose the nuclei are partitioned into equivalence classes such that n_1 nuclei are in the first equivalence class, n_2 nuclei in the second equivalence class ..., n_m nuclei in the m th equivalence class. The Euclidian distance group G of the molecule must be a subgroup of $S_{n_1} \times S_{n_2} \times \dots \times S_{n_m}$, where S_{n_i} is a permutation group containing $n_i!$ elements. That is

$$G \subseteq S_{n_1} \times S_{n_2} \times \dots \times S_{n_m}$$

$$\sum_{i=1}^n n_i$$

where m is the number of equivalence classes.

As a first step, the code that we have developed generates the nuclear equivalence classes from the k th order Euclidian distance algorithm. Then it generates all $n_1!n_2! \dots n_m!$ permutations of n nuclei. The basic the condition for the permutation to be in the Euclidian distance group, namely, $\mathbf{D}_{p_i p_j} = \mathbf{D}_{ij}$ is checked for each of the permutations without performing matrix multiplications. The properties of a group such as closure and inverse can be used to accelerate the performance of the code.

3. RESULTS AND DISCUSSION

The above algorithms were implemented on a computer using the FORTRAN '77 language. The execution was tested on an IBM RS/6000 580 workstation for several molecules. We discuss below a few of these examples. As a first example, let us consider the ferrocene molecule in the eclipsed conformation. The salient steps of our computations are shown in Table 1. As seen from this table, the code first lists the lower triangle of the Euclidian matrix. There is an option to scale the matrix elements by a scaling factor, but this was not invoked in this case. Following this, all permutations which preserve the Euclidian distance matrix are listed in Table 1. The code finds 20 permutations which constitute the Euclidian distance group. Note that the point group of this molecule is D_{5h} , and all operations generate unique nuclear permutations. We could have cases where improper rotational operations do not generate new nuclear permutations.

Table 2 illustrates the computed results for the benzene molecule. This is an interesting molecule since the improper rotational operations do not generate new permutational operations. As seen from Table 2, the code generates 12 permutations that preserve the Euclidian distance matrix of benzene. These permutations span a group which is isomorphic to the D_6 group. The horizontal mirror plane generates the same nuclear permutation as the identity operation. This is a quick test to see if the permutations

Table 1. Computation of the Euclidian Distance Group of the Eclipsed Form of Ferrocene

Lower Triangle of the Euclidian Matrix									
0.0000									
1.0000	0.0000								
1.6180	1.0000	0.0000							
1.6180	1.6180	1.0000	0.0000						
1.0000	1.6180	1.6180	1.0000	0.0000					
2.0000	2.2361	2.5726	2.5726	2.2361	0.0000				
2.2361	2.0000	2.2361	2.5726	2.5726	1.0000	0.0000			
2.5726	2.2361	2.0000	2.2361	2.5726	1.6180	1.0000	0.0000		
2.5726	2.5726	2.2361	2.0000	2.2361	1.6180	1.6180	1.0000	0.0000	
2.2361	2.5726	2.5726	2.2361	2.0000	1.0000	1.6180	1.6180	1.0000	0.0000
Permutations in the Permutation-Inversion Group									
1	2	3	4	5	6	7	8	9	10
4	3	2	1	5	9	8	7	6	10
10	9	8	7	6	5	4	3	2	1
7	8	9	10	6	2	3	4	5	1
8	9	10	6	7	3	4	5	1	2
6	10	9	8	7	1	5	4	3	2
9	10	6	7	8	4	5	1	2	3
7	6	10	9	8	2	1	5	4	3
8	7	6	10	9	3	2	1	5	4
10	6	7	8	9	5	1	2	3	4
6	7	8	9	10	1	2	3	4	5
9	8	7	6	10	4	3	2	1	5
5	4	3	2	1	10	9	8	7	6
2	3	4	5	1	7	8	9	10	6
3	4	5	1	2	8	9	10	6	7
1	5	4	3	2	6	10	9	8	7
4	5	1	2	3	9	10	6	7	8
2	1	5	4	3	7	6	10	9	8
5	1	2	3	4	10	6	7	8	9
3	2	1	5	4	8	7	6	10	9
no. of elements in the permutational group 20									

Table 2. Computation of the Euclidian Distance Group of Benzene

Permutations in the Permutation-Inversion Group					
1	2	3	4	5	6
5	4	3	2	1	6
2	3	4	5	6	1
6	5	4	3	2	1
1	6	5	4	3	2
3	4	5	6	1	2
4	5	6	1	2	3
2	1	6	5	4	3
5	6	1	2	3	4
3	2	1	6	5	4
6	1	2	3	4	5
4	3	2	1	6	5
no. of permutations in the group 12					

generated by the improper axes of rotations are already present in the permutational group of proper rotational operations. All improper rotational axes of the D_{6h} point group of benzene thus generate the same permutations already generated by the proper rotational axes. Consequently, the Euclidian distance group of the benzene molecule contains only half the number of elements in the point group.

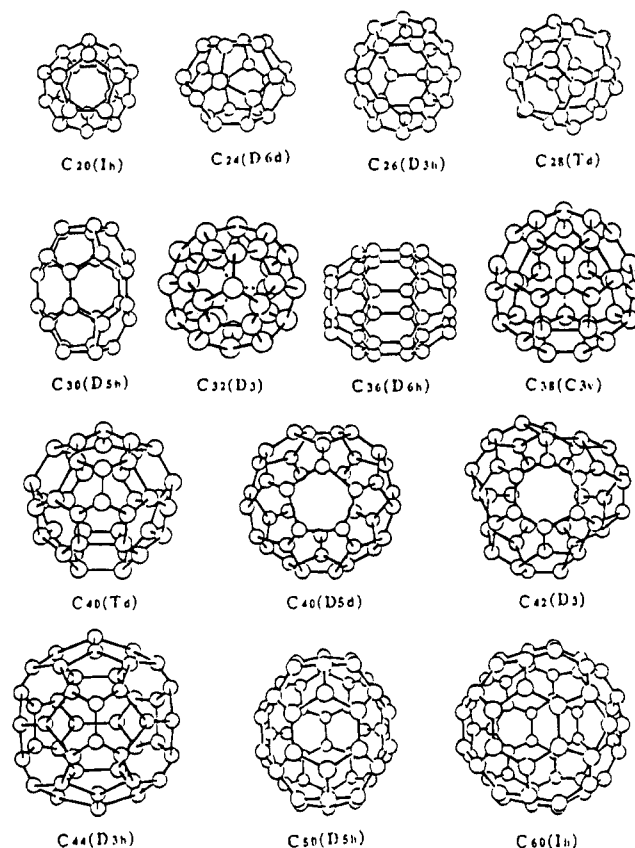
The cube structure offers considerable scope for critical testing of the code developed here. Table 3 shows the output of our code. The vertices of the cube were considered for the generation of the Euclidian distance matrix and the Euclidian distance group. As seen from Table 3, the edges of the cubes are defined to have 2 units of length. As indicated before, the Euclidian distance matrix can be scaled by any scaling factor, and the Euclidian distance group is invariant to such a scaling scheme. The code generates 48 permutations which constitute a group isomorphic to the octahedral point group O_h . In the case of cube, improper

Table 3. Computation of the Symmetry of the Cube Expressed as the Euclidian Distance Group

Upper Triangle of the Euclidian Matrix of the Cube							
0.0000							
2.0000	0.0000						
2.8284	2.0000	0.0000					
2.0000	2.8284	2.0000	0.0000				
2.8284	3.4641	2.8284	2.0000	0.0000			
3.4641	2.8284	2.0000	2.8284	2.0000	0.0000		
2.8284	2.0000	2.8284	3.4641	2.8284	2.0000	0.0000	
2.0000	2.8284	3.4641	2.8284	2.0000	2.8284	2.0000	0.0000
Permutations of the Vertices that Preserve the Euclidian Matrix							
1	2	3	4	5	6	7	8
5	6	3	4	1	2	7	8
5	4	3	6	7	2	1	8
7	2	3	6	5	4	1	8
7	6	3	2	1	4	5	8
1	4	3	2	7	6	5	8
2	7	6	3	4	5	8	1
4	5	6	3	2	7	8	1
4	3	6	5	8	7	2	1
8	7	6	5	4	3	2	1
2	3	6	7	8	5	4	1
8	5	6	7	2	3	4	1
1	8	5	4	3	6	7	2
3	6	5	4	1	8	7	2
7	8	5	6	3	4	1	2
3	4	5	6	7	8	1	2
7	6	5	8	1	4	3	2
1	4	5	8	7	6	3	2
6	5	8	7	2	1	4	3
2	1	8	7	6	5	4	3
2	7	8	1	4	5	6	3
4	5	8	1	2	7	6	3
4	1	8	5	6	7	2	3
6	7	8	5	4	1	2	3
5	6	7	8	1	2	3	4
1	2	7	8	5	6	3	4
1	8	7	2	3	6	5	4
3	6	7	2	1	8	5	4
3	2	7	6	5	8	1	4
5	8	7	6	3	2	1	4
6	3	2	7	8	1	4	5
8	1	2	7	6	3	4	5
8	7	2	1	4	3	6	5
4	3	2	1	8	7	6	5
6	7	2	3	4	1	8	5
4	1	2	3	6	7	8	5
5	4	1	8	7	2	3	6
7	2	1	8	5	4	3	6
3	4	1	2	7	8	5	6
7	8	1	2	3	4	5	6
3	2	1	4	5	8	7	6
5	8	1	4	3	2	7	6
2	3	4	1	8	5	6	7
8	5	4	1	2	3	6	7
2	1	4	3	6	5	8	7
6	5	4	3	2	1	8	7
6	3	4	5	8	1	2	7
8	1	4	5	6	3	2	7
total no. of members in the permutational group 48							

rotational operations generate new permutations, and thus all 48 point group operations generate different permutational representations.

The code developed here can be applied to more complex structures such as the fullerene clusters. Figure 2 shows several fullerene structures some of which will be considered subsequently. However, for fullerenes it is more convenient to define the Euclidian distance matrices using the distances between the rings. This is primarily because the number of vertices of fullerenes is usually larger than the number of rings. A related matrix in graph theory is called the ring

**Figure 2.** Structures of some fullerenes.

adjacency matrix. The use of ring adjacency matrices results in significant simplification for fullerenes.

Recall that fullerenes are closed-cage carbon clusters containing 12 pentagons and any number of hexagons. The Euler rule predicts that the number of hexagons in a fullerene is given by

$$h = (n - 20)/2$$

Hence there are fewer hexagons than pentagons for smaller fullerenes, while there are more hexagons than pentagons for fullerenes larger than C_{44} . Thus the use of Euclidian distances between hexagons leads to rapid perception of symmetry for fullerenes smaller than C_{44} , while the use of the ring Euclidian matrix between the pentagons leads to rapid perception of symmetry for larger fullerenes. It is this interesting that the order of the ring Euclidian matrix is at the most 12×12 for all fullerenes. Randic²⁰ has used the topological ring adjacency matrix for characterizing fullerenes. Further simplification can be accomplished in the symmetry perception algorithm if one uses higher order ring Euclidian matrices, but this was not implemented in the current code. The code developed here was aimed at applications to any structure. However, it can be applied to fullerenes as well without much difficulty.

Table 4 shows the output of our code for the C_{24} fullerene structure which contains 12 pentagons and two hexagons. The code used the ring Euclidian matrix restricted to pentagons, and thus the Euclidian matrix is of order 12×12 . The Euclidian distances shown in Table 4 are the Euclidian distances between the centers of pentagons. The lower triangle of the ring Euclidian matrix is shown in Table 4 with the neighboring pentagons exhibiting unit distances. The Euclidian distance group of C_{24} contains 24 permutations

Table 4. The Symmetry Group of the C_{24} Fullerene Using the Euclidian Ring Matrix Restricted to Pentagons

0.0000												
1.0000	0.0000											
1.7321	1.0000	0.0000										
2.0000	1.7321	1.0000	0.0000									
1.7321	2.0000	1.7321	1.0000	0.0000								
1.0000	1.7321	2.0000	1.7321	1.0000	0.0000							
2.0659	2.0659	2.4495	2.7807	2.7807	2.4495	0.0000						
2.4495	2.0659	2.0659	2.4495	2.7807	2.7807	1.0000	0.0000					
2.7807	2.4495	2.0659	2.0659	2.4495	2.7807	1.7321	1.0000	0.0000				
2.7807	2.7807	2.4495	2.0659	2.0659	2.4495	2.0000	1.7321	1.0000	0.0000			
2.4495	2.7807	2.7807	2.4495	2.0659	2.0659	1.7321	2.0000	1.7321	1.0000	0.000		
2.0659	2.4495	2.7807	2.7807	2.4495	2.0659	1.0000	1.7321	2.0000	1.7321	1.0000	0.0000	
Permutations in the Euclidian Distance Group												
1	2	3	4	5	6	7	8	9	10	11	12	
6	5	4	3	2	1	11	10	9	8	7	12	
12	11	10	9	8	7	6	5	4	3	2	1	
7	8	9	10	11	12	2	3	4	5	6	1	
8	9	10	11	12	7	3	4	5	6	1	2	
7	12	11	10	9	8	1	6	5	4	3	2	
9	10	11	12	7	8	4	5	6	1	2	3	
8	7	12	11	10	9	2	1	6	5	4	3	
10	11	12	7	8	9	5	6	1	2	3	4	
9	8	7	12	11	10	3	2	1	6	5	4	
10	9	8	7	12	11	4	3	2	1	6	5	
11	12	7	8	9	10	6	1	2	3	4	5	
12	7	8	9	10	11	1	2	3	4	5	6	
11	10	9	8	7	12	5	4	3	2	1	6	
1	6	5	4	3	2	12	11	10	9	8	7	
2	3	4	5	6	1	8	9	10	11	12	7	
3	4	5	6	1	2	9	10	11	12	7	8	
2	1	6	5	4	3	7	12	11	10	9	8	
4	5	6	1	2	3	10	11	12	7	8	9	
3	2	1	6	5	4	8	7	12	11	10	9	
5	6	1	2	3	4	11	12	7	8	9	10	
4	3	2	1	6	5	9	8	7	12	11	10	
6	1	2	3	4	5	12	7	8	9	10	11	
5	4	3	2	1	6	10	9	8	7	12	11	
total no. of members in the Euclidian distance group 24												

shown in Table 4. The resulting group is isomorphic to the D_{6d} point group of the C_{24} fullerene cluster.

The C_{28} fullerene (Figure 2) contains four hexagons and 12 pentagons. The relationship between the hexagons suffices to generate the Euclidian distance group of the C_{28} fullerene. Table 5 shows our computations of the Euclidian distance group which is also isomorphic to the permutation-inversion group. As seen from Table 5, the Euclidian distances between the hexagons are computed in a scale where the distance between the centers of hexagons is $2\sqrt{2}$. The code generates 24 permutations which constitute a group isomorphic with the tetrahedral point group T_d . Although the permutations are enumerated in terms of the hexagonal rings, they can be converted into permutations of the vertices or the edges. This requires the Euclidian matrix of the vertices (nuclei) or the edges (bonds).

As a last example let us consider the C_{60} buckminsterfullerene. In this case it is convenient to use the Euclidian ring matrix for the pentagons since there are fewer pentagons than hexagons in the structure. Defining the Euclidian distances of neighboring pentagons as unities, Table 6 shows the lower triangle of the ring Euclidian distance matrix of pentagons. As seen from Table 6, the code generates 120 permutations isomorphic with the icosahedral point group I_h . It is noteworthy that the problem of computer perception of the symmetry of the C_{60} buckminsterfullerene would have been considerably more complex, if one used the Euclidian distance matrix of all 60 atoms. However, powers of either the Euclidian distance matrix of the vertices or rings yield

Table 5. Computation of the Euclidian Distance of the C_{28} Fullerene Using the Ring Euclidian Matrix of Hexagons

Ring Euclidian Matrix of Hexagons			
0.0000			
2.8284	0.0000		
2.8284	2.8284	0.0000	
2.8284	2.8284	2.8284	0.0000
Permutations in the Permutation-Inversion Group			
1	2	3	4
2	1	3	4
2	3	1	4
3	2	1	4
3	1	2	4
1	3	2	4
4	3	2	1
3	4	2	1
2	4	3	1
4	2	3	1
3	2	4	1
2	3	4	1
1	3	4	2
3	1	4	2
3	4	1	2
4	3	1	2
4	1	3	2
1	4	3	2
4	1	2	3
2	1	4	3
1	2	4	3
4	2	1	3
2	4	1	3
no. of elements in the permutational group 24			

Table 6. Computation of the Permutation-Inversion Group of the C₆₀ Buckminsterfullerene Using the Euclidian Ring Matrix of Pentagons

Euclidian Ring Matrix of Pentagons											
0.0000											
1.0000	0.0000										
1.0000	1.0000	0.0000									
1.0000	1.6180	1.0000	0.0000								
1.0000	1.6180	1.6180	1.0000	0.0000							
1.0000	1.0000	1.6180	1.6180	1.0000	0.0000						
1.6180	1.9021	1.6180	1.0000	1.0000	1.6180	0.0000					
1.6180	1.6180	1.9021	1.6180	1.0000	1.0000	1.0000	0.0000				
1.6180	1.0000	1.6180	1.9021	1.6180	1.0000	1.6180	1.0000	0.0000			
1.6180	1.0000	1.0000	1.6180	1.9021	1.6180	1.6180	1.6180	1.0000	0.0000		
1.6180	1.6180	1.0000	1.0000	1.6180	1.9021	1.0000	1.6180	1.6180	1.0000	0.0000	
1.9021	1.6180	1.6180	1.6180	1.6180	1.6180	1.0000	1.0000	1.0000	1.0000	1.0000	0.0000
Permutations in the Permutation-Inversion Group											
1	2	3	4	5	6	7	8	9	10	11	12
1	5	4	3	2	6	10	9	8	7	11	12
1	6	5	4	3	2	11	10	9	8	7	12
1	3	4	5	6	2	8	9	10	11	7	12
1	4	5	6	2	3	9	10	11	7	8	12
1	2	6	5	4	3	7	11	10	9	8	12
1	5	6	2	3	4	10	11	7	8	9	12
1	3	2	6	5	4	8	7	11	10	9	12
1	6	2	3	4	5	11	7	8	9	10	12
1	4	3	2	6	5	9	8	7	11	10	12
12	8	9	10	11	7	3	4	5	6	2	1
12	11	10	9	8	7	6	5	4	3	2	1
12	7	11	10	9	8	2	6	5	4	3	1
12	9	10	11	7	8	4	5	6	2	3	1
12	10	11	7	8	9	5	6	2	3	4	1
12	8	7	11	10	9	3	2	6	5	4	1
12	11	7	8	9	10	6	2	3	4	5	1
12	9	8	7	11	10	4	3	2	6	5	1
12	10	9	8	7	11	5	4	3	2	6	1
12	7	8	9	10	11	2	3	4	5	6	1
7	5	8	12	11	4	10	3	1	6	9	2
7	11	12	8	5	4	6	1	3	10	9	2
7	8	12	11	4	5	3	1	6	9	10	2
7	4	11	12	8	5	9	6	1	3	10	2
7	11	4	5	8	12	6	9	10	3	1	2
7	8	5	4	11	12	3	10	9	6	1	2
7	5	4	11	12	8	10	9	6	1	3	2
7	12	11	4	5	8	1	6	9	10	3	2
7	12	8	5	4	11	1	3	10	9	6	2
7	4	5	8	12	11	9	10	3	1	6	2
8	6	9	12	7	5	11	4	1	2	10	3
8	7	12	9	6	5	2	1	4	11	10	3
8	5	7	12	9	6	10	2	1	4	11	3
8	9	12	7	5	6	4	1	2	10	11	3
8	9	6	5	7	12	4	11	10	2	1	3
8	7	5	6	9	12	2	10	11	4	1	3
8	12	9	6	5	7	1	4	11	10	2	3
8	5	6	9	12	7	10	11	4	1	2	3
8	12	7	5	6	9	1	2	10	11	4	3
8	6	5	7	12	9	11	10	2	1	4	3
9	6	8	12	10	2	11	3	1	5	7	4
9	10	12	8	6	2	5	1	3	11	7	4
9	2	10	12	8	6	7	5	1	3	11	4
9	8	12	10	2	6	3	1	5	7	11	4
9	10	2	6	8	12	5	7	11	3	1	4
9	8	6	2	10	12	3	11	7	5	1	4
9	12	10	2	6	8	1	5	7	11	3	4
9	6	2	10	12	8	11	7	5	1	3	4
9	2	6	8	12	10	7	11	3	1	5	4
9	12	8	6	2	10	1	3	11	7	5	4
10	3	2	9	12	11	8	7	4	1	6	5
10	12	9	2	3	11	1	4	7	8	6	5
10	3	11	12	9	2	8	6	1	4	7	5
10	9	12	11	3	2	4	1	6	8	7	5
10	2	9	12	11	3	7	4	1	6	8	5
10	11	12	9	2	3	6	1	4	7	8	5
10	11	3	2	9	12	6	8	7	4	1	5
10	9	2	3	11	12	4	7	8	6	1	5
10	2	3	11	12	9	7	8	6	1	4	5
10	12	11	3	2	9	1	6	8	7	4	5
11	12	7	4	3	10	1	2	9	8	5	6

Table 6 (Continued)

Permutations in the Permutation-Inversion Group											
11	3	4	7	12	10	8	9	2	1	5	6
11	4	7	12	10	3	9	2	1	5	8	6
11	10	12	7	4	3	5	1	2	9	8	6
11	7	12	10	3	4	2	1	5	8	9	6
11	3	10	12	7	4	8	5	1	2	9	6
11	10	3	4	7	12	5	8	9	2	1	6
11	7	4	3	10	12	2	9	8	5	1	6
11	12	10	3	4	7	1	5	8	9	2	6
11	4	3	10	12	7	9	8	5	1	2	6
2	6	1	3	10	9	11	12	8	5	4	7
2	10	3	1	6	9	5	8	12	11	4	7
2	3	1	6	9	10	8	12	11	4	5	7
2	9	6	1	3	10	4	11	12	8	5	7
2	1	6	9	10	3	12	11	4	5	8	7
2	10	9	6	1	3	5	4	11	12	8	7
2	9	10	3	1	6	4	5	8	12	11	7
2	1	3	10	9	6	12	8	5	4	11	7
2	6	9	10	3	1	11	4	5	8	12	7
2	3	10	9	6	1	8	5	4	11	12	7
3	2	1	4	11	10	7	12	9	6	5	8
3	11	4	1	2	10	6	9	12	7	5	8
3	4	1	2	10	11	9	12	7	5	6	8
3	10	2	1	4	11	5	7	12	9	6	8
3	10	11	4	1	2	5	6	9	12	7	8
3	1	4	11	10	2	12	9	6	5	7	8
3	11	10	2	1	4	6	5	7	12	9	8
3	1	2	10	11	4	12	7	5	6	9	8
3	4	11	10	2	1	9	6	5	7	12	8
3	2	10	11	4	1	7	5	6	9	12	8
4	5	1	3	11	7	10	12	8	6	2	9
4	11	3	1	5	7	6	8	12	10	2	9
4	7	5	1	3	11	2	10	12	8	6	9
4	3	1	5	7	11	8	12	10	2	6	9
4	1	5	7	11	3	12	10	2	6	8	9
4	11	7	5	1	3	6	2	10	12	8	9
4	7	11	3	1	5	2	6	8	12	10	9
4	1	3	11	7	5	12	8	6	2	10	9
4	5	7	11	3	1	10	2	6	8	12	9
4	3	11	7	5	1	8	6	2	10	12	9
5	4	7	8	6	1	9	2	3	11	12	10
5	6	8	7	4	1	11	3	2	9	12	10
5	8	6	1	4	7	3	11	12	9	2	10
5	4	1	6	8	7	9	12	11	3	2	10
5	7	4	1	6	8	2	9	12	11	3	10
5	6	1	4	7	8	11	12	9	2	3	10
5	7	8	6	1	4	2	3	11	12	9	10
5	1	6	8	7	4	12	11	3	2	9	10
5	8	7	4	1	6	3	2	9	12	11	10
5	1	4	7	8	6	12	9	2	3	11	10
6	8	9	2	1	5	3	4	7	12	10	11
6	1	2	9	8	5	12	7	4	3	10	11
6	5	8	9	2	1	10	3	4	7	12	11
6	2	9	8	5	1	7	4	3	10	12	11
6	5	1	2	9	8	10	12	7	4	3	11
6	9	2	1	5	8	4	7	12	10	3	11
6	2	1	5	8	9	7	12	10	3	4	11
6	8	5	1	2	9	3	10	12	7	4	11
6	9	8	5	1	2	4	3	10	12	7	11
6	1	5	8	9	2	12	10	3	4	7	11

no. of elements in the permutation-inversion group 120

additional information which can be exploited in accelerating computer perception of symmetry.

4. CONCLUSIONS

In this study we developed a code and algorithms for the machine perception of molecular symmetry. The code uses the Euclidian distance matrices which are invariant to proper and improper rotations, translations, scaling, and other operations. The equivalence classes of nuclei generated by the powers of the Euclidian distance matrices were used to accelerate the machine perception of molecular symmetry.

We used an algorithm based on memory manipulation rather than matrix multiplication for rapid machine perception of symmetry.

The code could be applied to the fullerene clusters through the use of ring Euclidian matrices. It was shown that use of such matrices which define the Euclidian distance relationships for pentagons or hexagons leads to rapid machine perception of the symmetry of the C_{60} buckminsterfullerene and C_{24} and C_{28} fullerenes.

The code generates permutations of the nuclei or rings that leave the Euclidian distance matrix of the structure under

investigation invariant. These permutations were shown to constitute a group called the Euclidian distance group which is isomorphic to the permutation-inversion group of Longuet-Higgins¹ in the event the improper rotational operations generate permutations that are not already contained in the permutational subgroup generated by the proper rotational operations. Otherwise the Euclidian distance group generates the unique permutations generated by the proper rotational operations of the traditional point group of the molecule.

The code developed here generates the unique permutations contained in the permutation-inversion group of the rigid molecule from which several other useful functions and structures can be obtained. For example, the cycle index of a group and the generalized character cycle indices can be readily obtained. These indices find several applications in molecular spectroscopy, NMR spectroscopy, ESR spectroscopy, and so on. The isomers of polysubstituted structures including stereoisomers derived by substitution of the parent structure can be readily obtained from these indices. The permutations can also be readily grouped into conjugacy classes.

REFERENCES AND NOTES

- (1) Longuet-Higgins, H. C. The symmetry Group of a Non-rigid Molecule. *Molecular Phys.* **1963**, *6*, 445.
- (2) Balasubramanian, K. Applications of Combinatorics and Graph Theory to Spectroscopy and Quantum Chemistry. *Chem. Rev.* **1985**, *85*, 599–618.
- (3) Balasubramanian, K. Computational Techniques for the Automorphism Groups of Weighted Graphs. *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 1146–1150.
- (4) Balasubramanian, K. Computational Techniques for the Automorphism Groups of Graphs. *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 621.
- (5) Razinger, M.; Balasubramanian, K.; Munk, M. E. Graph Automorphism Perception Algorithms in Computer-Enhanced Structure Elucidation. *J. Chem. Inf. Comput. Sci.* **1993**, *33*, 197–201.
- (6) Balasubramanian, K. Symmetry Groups of Chemical Graphs. *Int. J. Quantum Chem.* **1982**, *21*, 411–418.
- (7) Liu, X.; Balasubramanian, K.; Munk, M. E. Computational Techniques for Vertex Partitioning of Graphs. *J. Chem. Inf. Comput. Sci.* **1990**, *30*, 263–269.
- (8) King, R. B. The Bonding Topology of Polyhedral Molecules. In *Chemical Applications of Topology and Graph Theory*; King, R. B., Ed.; Studies in Physical and Theoretical Chemistry; Elsevier: Amsterdam, 1983; Vol. 28, pp 108–122.
- (9) Randić, M. Symmetry Properties of Graphs of Interest in Chemistry II. Desargues-Levi Graph. *Int. J. Quantum Chem.* **1979**, *15*, 663–682.
- (10) Randić, M.; Davis, M. I. Symmetry Properties of Chemical Graphs VI. Isomerizations of Octahedral Complexes. *Int. J. Quantum Chem.* **1984**, *26*, 69–89.
- (11) Balasubramanian, K. Graph Theoretical Perception of Molecular Symmetry. *Chem. Phys. Lett.* **1995**, *232*, 415–423.
- (12) Balasubramanian, K. Geometry-dependent Characteristic Polynomials of Molecular Structures. *Chem. Phys. Lett.* **1990**, *169*, 224–230.
- (13) Nikolić, S.; Trinajstić, N.; Mihalić, Z.; Carter, S. On the Geometric Distance Matrix and the Corresponding Structural Invariants of Molecular Systems. *Chem. Phys. Lett.* **1991**, *179*, 21–28.
- (14) Randić, M.; Jerman Blazić, B.; Trinajstić, N. Development of Three-dimensional Molecular Descriptors. *Comput. Chem.* **1990**, *14*, 237–246.
- (15) Randić, M.; Razinger, M. Molecular Topographic Indices. *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 140–147.
- (16) Balasubramanian, K. Combinatorial Methods in ESR Spectroscopy. *J. Magn. Reson.* **1991**, *91*, 45–56.
- (17) Balasubramanian, K. ESR Hyperfine Patterns for Radicals Derived from C₆₀ and C₇₀. *Chem. Phys. Lett.* **1993**, *210*, 153.
- (18) Balasubramanian, K. Combinatorics of NMR and ESR Spectral Simulations. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 296–298.
- (19) Balasubramanian, K. The Combinatorics of Symmetry-Adaptation. *Theor. Chim. Acta* **1981**, *59*, 47–54.
- (20) Randić, M. Characterization of Fullerenes. *Fullerene Sci., Tech.* **1994**, *2*, 427–444.

CI950026N