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COMPUTER GENERATION OF THE SYMMETRY ELEMENTS OF NON-RIGID MOLECULES

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Computer Generation of the Symmetry Elements of Non-rigid Molecules

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Abstract

Algorithms and computer programs are developed for generating the symmetry elements of non-rigid molecules. These programs are based on the wreath product formalism for the symmetry groups of non-rigid molecules developed by the present author. Several examples are given to illustrate the procedures. Applications to weakly bound van der Waal complexes synthesized by supersonic beam expansion are also presented.

I. Introduction

The symmetry groups of non-rigid molecules contain permutation and inversion operations (PI operations) induced by large amplitude motions. This permutation-inversion group approach to describe the symmetry of non-rigid molecules was essentially formulated by Longuet-Higgins.[1] Since this formulation several other authors[2-9] have developed equivalent formulations. The present author[10-12] has shown that the symmetry groups of molecules which exhibit internal rotations can be represented by wreath product groups or in general, generalized wreath product groups. The symmetry groups of non-rigid molecules have several applications in chemical physics. A review of these applications can be found in the author's article[13] and several other articles that appear in Ref. 13.

The symmetry of permutation processes in non-rigid molecules can be represented by associated diagrams known as isomerization graphs. Randić,[14,16] Randić and Klein[17] and Balaban[18,19] studied the symmetry properties of these graphs. The symmetry groups of some of these graphs are wreath product groups. For example, the symmetry group of the isomerization graph of propane is a generalized wreath product group as shown by Randić[16] recently. A computer program to generate the symmetry elements of these groups will be of great use in understanding these permutational processes.

The number of symmetry elements of non-rigid molecules increase in an exponential order, exponent being the number of internal rotors in the molecule. Even a simple non-rigid molecule like isobutane has 162 symmetry elements. Therefore, it will be advantageous to have a computer program that will generate the symmetry elements of non-rigid molecules. We develop a computer program which generates the symmetry

elements of non-rigid molecules (with symmetry groups that can be embedded into wreath products) from the symmetry groups of much smaller orders. For example, the symmetry group of isobutane can be generated by this program using the symmetry elements of C_{3v} group. The wreath product groups have several elegant applications to NMR spectroscopy,[20-22] nuclear spin statistics,[23,24] symmetry of chemical graphs,[25] CI calculations[26] etc. For these reasons we undertake the present investigation.

Section II describes the basic algorithm, computer programs and illustrative examples. Section III gives applications such as application to symmetry groups of weakly bound van der Waal complexes generated by supersonic molecular beam expansion.

II. Computer Generation of the Symmetry Elements of Non-rigid Molecules

A. Preliminaries and Definitions

Before we consider computer algorithms we will first review our formulation of the symmetry groups of non-rigid molecules as generalized wreath product groups. The present author[10,12] showed that the symmetry groups of non-rigid molecules exhibiting internal rotation are expressible as wreath product groups.

Consider the non-rigid hydrazine molecule. This molecule is non-rigid in that at room temperature the protons of each nitrogen atom are rapidly permuted by a twisting operation. This non-rigid molecule can be modeled by a particle-in-box model as shown in Figure 1. The protons attached to each nitrogen atom can be thought of as particles in a box. The particles in each box can be permuted by the twisting operation. The boxes can also be permuted as a consequence of the symmetry of the rigid molecule. The resulting operations generated by switching the particles and boxes are shown in Figure 1. Suppose G is the

permutation group of boxes and H is the permutation group of particles in each box then the permutation group of all the particles and boxes is simply the wreath product of G and H, denoted as G[H]. It is formally defined as follows. Let Ω be the set $\Omega = \{1,2,...n\}$. Let G be a permutation group acting on Ω and let H be another permutation group. Then the wreath product G[H] is the set

$$\{(g;\pi) \mid \pi:\Omega \to H,\ g\varepsilon G\}$$

such that the product of two maps π_1 and π_2: $\Omega \to H$ is defined as

$$\pi_1 \cdot \pi_2(i) = \pi_1(i)\ \pi_2(i), \qquad i\varepsilon\Omega,$$

and the product of $(g_1;\pi_1)$ and $(g_2;\pi_2)$ is defined as

$$(g_1;\pi_1)(g_2;\pi_2) = (g_1g_2;\pi_1\pi_{2g_1}).$$

The map π_{2g_1} is defined as follows:

$$\pi_{2g_1}(i) = \pi_2(g_1^{-1}i), \qquad i\varepsilon\Omega.$$

It can be shown that the above set forms a group and it is called the wreath product of G and H. For the hydrazine molecule G and H are both the symmetric group S_2 so that the permutation group of the non-rigid molecule is $S_2[S_2]$. Several illustrative examples of wreath product groups can be found elsewhere.[10,12]

Let H_i be the group defined as follows.

$$H_i = \{(e;\pi) \mid \pi(j) = {}^1H,\ j \neq i\}$$

where ${}^1H$ is the identity of H. Note that H_i is isomorphic to H. Let G' be the group defined as follows.

$$G' = \{(g;e') \mid e'(j) = {}^{1}H \ \forall j\}.$$

Then the wreath product of G[H] has the following permutation representation.

$$G[H] = (H_1 \times H_2 \times \ldots \times H_n) \quad G'$$

where $n = |\Omega|$, the number of elements in the set Ω.

In this paper we develop computer programs which generate the symmetry elements of non-rigid molecules using the wreath product formalism.

We will use the following notation for a permutation. Any permutation of n objects is characterized by a 2 x n matrix in which the first row the elements 1,2,...n are in their natural position and the second row contains the elements to which they are permuted. To illustrate, the permutation (123) takes the following form.

$$(123) : \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}$$

An element i in the first row goes to the element P(i) in the second row. We will use the right-to-left multiplication convention. For example, the product of (123) and (12) is shown below in this convention.

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}\begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix}$$

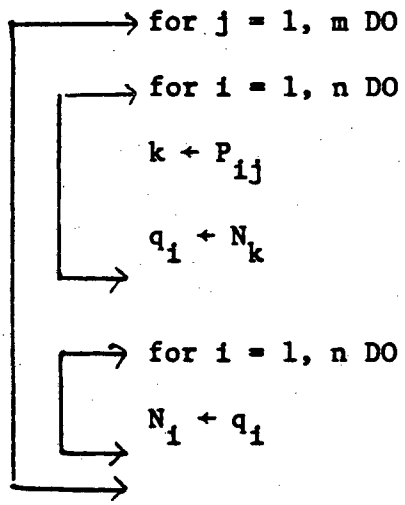
For the sake of convenience we will omit the first row in which the column j is always j. For example, the permutation (123) can simply be denoted as 231.

B. Algorithms

This section outlines the basic algorithms used to generate the symmetry elements of non-rigid molecules. First we describe the algorithm PROPER which generates the product of m permutations of the same length n. Let $\{P_{ij}\}$ (j=1,m; i=1,n) be the set of m permutations

Algorithm Proper.

Initialise: $N_i \leftarrow i$, for $i = 1,n$.



The final array $(q_i)(i=1,n)$ obtained after the execution of the algorithm gives the permutation which is the product of m permutations in the array $((P_{ij}))$.

We will now illustrate this algorithm with an example of product of two permutations 231 and 213 used in an earlier example. Thus m and n are 2 and 3 respectively. The array N is initialized to 123. With this value the various steps of the algorithm are now executed.

P1: $j = 1$

$$i = 1 \cdot k = P_{11} = 2 \cdot q_1 = N_2 = 2$$

$$i = 2 \cdot k = P_{21} = 3 \cdot q_2 = N_3 = 3$$

$$i = 3 \cdot k = P_{31} = 1 \cdot q_3 = N_1 = 1$$

$$N_1 = q_1 = 2 \cdot N_2 = q_2 = 3 \cdot N_3 = q_3 = 1$$

P2: $j = 2$

$$i = 1 \cdot k = P_{12} = 2 \cdot q_1 = N_2 = 3$$

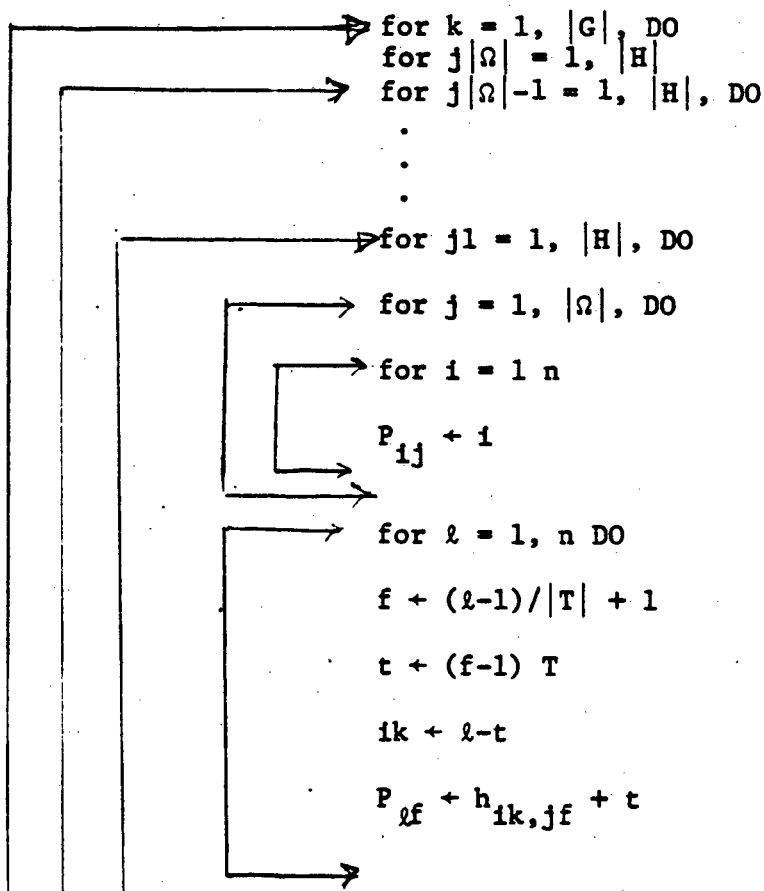
$$i = 2 \cdot k = P_{22} = 1 \cdot q_2 = N_1 = 2$$

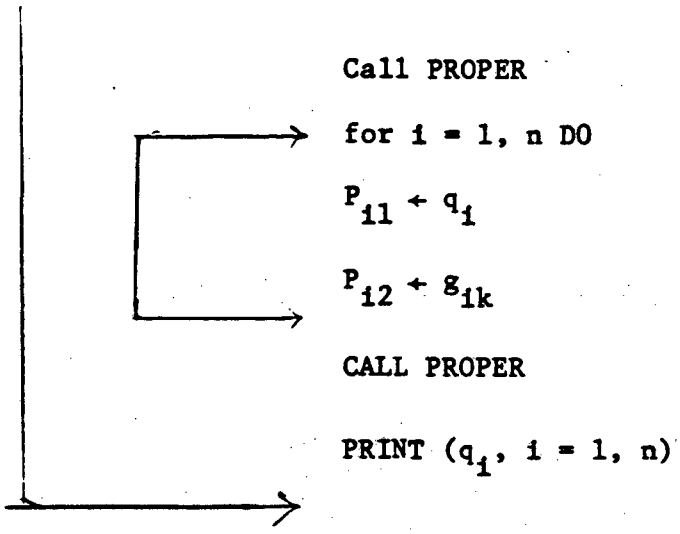
$$i = 3 \cdot k = P_{32} = 3 \cdot q_3 = N_3 = 1$$

$$N_1 = 3 \quad N_2 = 2 \quad N_3 = 1$$

The final result is contained in the array (q) which is 321. Thus the product of two permutations 231 and 213 is 321. In cycle notation this corresponds to (123)(12)(3) = (13)(2).

Now we describe the algorithm WREATH which generates the elements of the symmetry group of the non-rigid molecule. Let G and H be the groups whose wreath product G[H] is under consideration. Let G act on Ω and H act on T. Let h_{ij} and g_{ij} be the permutations of G and H. Let |S| denote the number of elements in the set S. Let n be the total number of nuclei in the molecule.





The array (q_i) of length n printed every time is a permutation in the symmetry group of the non-rigid molecule.

The two algorithms described above can be coded into Fortran. A Fortran program obtained thus is shown in Table I. This program requires the elements of G' and H as input and it generates the elements of non-rigid molecules. The program can handle both permutation and permutation inversion operations. The program actually reads in the elements of G' (cf. sec DA) rather than G since this is more convenient. Nevertheless, G' is isomorphic to G. Table II gives the input description for this program.

We will now illustrate the use of this program with two examples. First consider the non-rigid isobutane molecule. The symmetry group of this molecule contains 162 operations. The input to generate the symmetry elements of this molecule is shown in Table III. The output corresponding to this input is shown in Table IV. Note that the tertiary proton (10) is not permuted by any operation of the symmetry group of the non-rigid molecule. Hence it is omitted from the list.

III. Applications

The programs described here have applications in several areas. Firstly, of course, in characterizing the symmetry of molecules exhibiting large amplitude motions, this program will be of potential use. This program will be of further use in computer generation of the character tables of the symmetry groups of non-rigid molecules, their projection operators, etc.

Topological representation of isomerization processes and the elucidation of modes of rearrangements etc. are of great interest to several workers like Randić, Klein, Balaban and the present author. The computer programs developed here could be used in listing the symmetry elements of the associated chemical graph.

Finally, we give an application to molecular beam deflection experiments of weakly bound van der Waal complexes. It is possible to generate weakly bound complexes of molecules like NH_3, H_2O, C_6H_6, etc. by a supersonic jet expansion.[27-29] Molecules created this way are non-rigid in that they exhibit rapid tunneling motions at room temperature since they are very weakly bound polymers. It is important to know the nature of their symmetry groups in order to analyze their spectra etc. We will use benzene dimer $(C_6H_6)_2$ as an example to illustrate the use of our program. Since the PI group of this molecule is a direct product of P and I groups we will use our computer program to generate only the elements of its permutation group. Table V shows the computer output for this molecule.

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PROGRAM WREATH 76/76 OPT=1 FTN 4.8+508/045

Table I. Computer Program for the Symmetry Elements of Non-rigid Molecules

```
      *DECK WREATH
            PROGRAM WREATH(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
            INTEGER PG(100,50),PH(10,100),P(100,10),INV(100),PPRO(1000),JL(
           C,TITLE(10)
            READ(5,80)(TITLE(I),I=1,10)
      80    FORMAT(10A8)
            WRITE(6,79)
      79    FORMAT(1H1)
            WRITE(6,80)(TITLE(I),I=1,10)
            WRITE(6,81)
      81    FORMAT(6X,*NO*,4X,*PI OPERATION*)
            READ(5,90)N,MODOM,MODT,MODH,MODG
      90    FORMAT(20I4)
            READ(5,90)((PG(I,J),I=1,N),J=1,MODG)
            READ(5,92)(INV(I),I=1,MODG)
      92    FORMAT(80A1)
            READ(5,90)((PH(I,J),I=1,MODT),J=1,MODH)
            DO 700 II=1,10
      700   JL(II)=1
            DO 850 J=1,MODOM
      850     JL(J)=MODH
            JL10=JL(10)$JL9=JL(9)$JL8=JL(8)$JL7=JL(7)$JL6=JL(6)$JL5=JL(5)
            JL4=JL(4)$JL3=JL(3)$JL2=JL(2)$JL1=JL(1)
            IND=0
            DO 200 K=1,MODG
            DO 100 J10=1,JL10
            DO 100 J9=1,JL9
            DO 100 J8=1,JL8
            DO 100 J7=1,JL7
            DO 100 J6=1,JL6
            DO 100 J5=1,JL5
            DO 100 J4=1,JL4
            DO 100 J3=1,JL3
            DO 100 J2=1,JL2
            DO 100 J1=1,JL1
            DO 800 J=1,MODOM
            DO 800 I=1,N
      800     P(I,J)=I
            DO 50 II=1,N
            IFACT=(II-1)/MODT+1
            IT=(IFACT-1)*MODT
            IK=II-IT
            GO TO(21,22,23,24,25,26,27,28,29,30)IFACT
      21    P(II,IFACT)=PH(IK,J1)+IT
            GO TO 50
      22    P(II,IFACT)=PH(IK,J2)+IT
            GO TO 50
      23    P(II,IFACT)=PH(IK,J3)+IT
            GO TO 50
      24    P(II,IFACT)=PH(IK,J4)+IT
            GO TO 50
      25    P(II,IFACT)=PH(IK,J5)+IT
            GO TO 50
      26    P(II,IFACT)=PH(IK,J6)+IT
            GO TO 50
```

PROGRAM WREATH 76/76 OPT=1 Table I (cont'd) FTN 4.8+508

```
            27    P(II,IFACT)=PH(IK,J7)+IT
                   GO TO 50
            28    P(II,IFACT)=PH(IK,J8)+IT
                   GO TO 50
            29    P(II,IFACT)=PH(IK,J9)+IT
                   GO TO 50
            30    P(II,IFACT)=PH(IK,J10)+IT
            50    CONTINUE
                  CALL PROPER(P,N,MODGM,PPRO)
                  DO 250 II=1,N
                  P(II,1)=PPRO(II)
            250    P(II,2)=PG(II,K)
                  CALL PROPER(P,N,2,PPRO)
                  IND=IND+1
                  WRITE(6,93)IND,INV(K),(PPRO(II),II=1,N)
            93    FORMAT(2X,I6,2X,A1,20I4)
            100    CONTINUE
            200    CONTINUE
                   STOP
                   END
```

SUBROUTINE PROPER 76/76 OPT=1 FTN 4.8+508/04

```
1           *DECK PROPER
            SUBROUTINE PROPER(P,N,JK,PPRO)
            INTEGER P(100,10),PPRO(1000),NPRO(1000)
            DO 50 I=1,N
5           50     NPRO(I)=I
             DO 200 J=1,JK
            DO 100 I=1,N
            100    PPRO(I)=NPRO(P(I,J))
            DO 150 I=1,N
10          150    NPRO(I)=PPRO(I)
            200    CONTINUE
            RETURN
             END
```

Table II. Input Description for the Program Wreath Which Generates the Symmetry Elements of Non-rigid Molecule

Card	Format	Input Variables	Description
1	10A8	Title	Alphanumeric title
2	20I4	N	Total number of Nuclei
		MODOM	$\|\Omega\|$
		MODT	$\|T\|$
		MODH	$\|H\|$
		MODG	$\|G\|$
3*	20I4	PG(I,J) J=1,|G|, I=1,N	Permutations of the group G'
4	80A1	INV(I), I=1, |G|	Inversion variable. If the i^{th} operation in G is a pure permutation INV(i) = blank. If it is a permutation-inversion operation INV(i) = *
5	20I4	PH(I,J), J=1,|H|, I=1,MODT	Permutations of the group H

* The elements of G and H may need more than one card, depending on the number of elements in them.

Table III. Input for Generating the Symmetry Elements of Non-rigid Isobutane

Card	
1	Symmetry Elements of Non-rigid Isobutane
2	9 3 3 3 6
3	1 2 3 4 5 6 7 8 9 4 5 6 7 8 9 1 2 3 7 8
4	9 1 2 3 4 5 6 7 9 8 4 6 5 1 3 2 1 3 2 7
5	9 8 4 6 5 4 6 5 1 3 6 7 9 8
6	␣ ␣ ␣ * * *†
7	1 2 3 2 3 1 3 1 2

† ␣ denotes blank.

SYMMETRY ELEMENTS OF NON-RIGID ISOBUTANE - Table IV

NO	OF OPERATION								
1	1	2	3	4	5	6	7	8	9
2	2	3	1	4	5	6	7	8	9
3	3	1	2	4	5	6	7	8	9
4	1	2	3	5	6	4	7	8	9
5	2	3	1	5	6	4	7	8	9
6	3	1	2	5	6	4	7	8	9
7	1	2	3	6	4	5	7	8	9
8	2	3	1	6	4	5	7	8	9
9	3	1	2	6	4	5	7	8	9
10	1	2	3	4	5	6	8	9	7
11	2	3	1	4	5	6	8	9	7
12	3	1	2	4	5	6	8	9	7
13	1	2	3	5	6	4	8	9	7
14	2	3	1	5	6	4	8	9	7
15	3	1	2	5	6	4	8	9	7
16	1	2	3	6	4	5	8	9	7
17	2	3	1	6	4	5	8	9	7
18	3	1	2	6	4	5	8	9	7
19	1	2	3	4	5	6	9	7	8
20	2	3	1	4	5	6	9	7	8
21	3	1	2	4	5	6	9	7	8
22	1	2	3	5	6	4	9	7	8
23	2	3	1	5	6	4	9	7	8
24	3	1	2	5	6	4	9	7	8
25	1	2	3	6	4	5	9	7	8
26	2	3	1	6	4	5	9	7	8
27	3	1	2	6	4	5	9	7	8
28	4	5	6	7	8	9	1	2	3
29	4	5	6	7	8	9	2	3	1
30	4	5	6	7	8	9	3	1	2
31	5	6	4	7	8	9	1	2	3
32	5	6	4	7	8	9	2	3	1
33	5	6	4	7	8	9	3	1	2
34	6	4	5	7	8	9	1	2	3
35	6	4	5	7	8	9	2	3	1
36	6	4	5	7	8	9	3	1	2
37	4	5	6	8	9	7	1	2	3
38	4	5	6	8	9	7	2	3	1
39	4	5	6	8	9	7	3	1	2
40	5	6	4	8	9	7	1	2	3
41	5	6	4	8	9	7	2	3	1
42	5	6	4	8	9	7	3	1	2
43	6	4	5	8	9	7	1	2	3
44	6	4	5	8	9	7	2	3	1
45	6	4	5	8	9	7	3	1	2
46	4	5	6	9	7	8	1	2	3
47	4	5	6	9	7	8	2	3	1
48	4	5	6	9	7	8	3	1	2
49	5	6	4	9	7	8	1	2	3
50	5	6	4	9	7	8	2	3	1
51	5	6	4	9	7	8	3	1	2
52	6	4	5	9	7	8	1	2	3
53	6	4	5	9	7	8	2	3	1
54	6	4	5	9	7	8	3	1	2
55	7	8	9	1	2	3	4	5	6
56	7	8	9	2	3	1	4	5	6
57	7	8	9	3	1	2	4	5	6
58	7	8	9	1	2	3	5	6	4
59	7	8	9	2	3	1	5	6	4

60		7	8	9	3	1	2	5	6	4
61		7	8	9	1	2	3	6	4	5
62		7	8	9	2	3	1	6	4	5
63		7	8	9	3	1	2	6	4	5
64		8	9	7	1	2	3	4	5	6
65		8	9	7	2	3	1	4	5	6
66		8	9	7	3	1	2	4	5	6
67		8	9	7	1	2	3	5	6	4
68		8	9	7	2	3	1	5	6	4
69		8	9	7	3	1	2	5	6	4
70		8	9	7	1	2	3	6	4	5
71		8	9	7	2	3	1	6	4	5
72		8	9	7	3	1	2	6	4	5
73		9	7	8	1	2	3	4	5	6
74		9	7	8	2	3	1	4	5	6
75		9	7	8	3	1	2	4	5	6
76		9	7	8	1	2	3	5	6	4
77		9	7	8	2	3	1	5	6	4
78		9	7	8	3	1	2	5	6	4
79		9	7	8	1	2	3	6	4	5
80		9	7	8	2	3	1	6	4	5
81		9	7	8	3	1	2	6	4	5
82	*	1	3	2	7	9	8	4	6	5
83	*	2	1	3	7	9	8	4	6	5
84	*	3	2	1	7	9	8	4	6	5
85	*	1	3	2	7	9	8	5	4	6
86	*	2	1	3	7	9	8	5	4	6
87	*	3	2	1	7	9	8	5	4	6
88	*	1	3	2	7	9	8	6	5	4
89	*	2	1	3	7	9	8	6	5	4
90	*	3	2	1	7	9	8	6	5	4
91	*	1	3	2	8	7	9	4	6	5
92	*	2	1	3	8	7	9	4	6	5
93	*	3	2	1	8	7	9	4	6	5
94	*	1	3	2	8	7	9	5	4	6
95	*	2	1	3	8	7	9	5	4	6
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97	*	1	3	2	8	7	9	6	5	4
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103	*	1	3	2	9	8	7	5	4	6
104	*	2	1	3	9	8	7	5	4	6
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106	*	1	3	2	9	8	7	6	5	4
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111	*	7	9	8	4	6	5	3	2	1
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113	*	7	9	8	5	4	6	2	1	3
114	*	7	9	8	5	4	6	3	2	1
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119	*	8	7	9	4	6	5	2	1	3
120	*	8	7	9	4	6	5	3	2	1
121	*	8	7	9	5	4	6	1	3	2

122	*	8	7	9	5	4	6	2	1	3
123	*	8	7	9	5	4	6	3	2	1
124	*	8	7	9	6	5	4	1	3	2
125	*	8	7	9	6	5	4	2	1	3
126	*	8	7	9	6	5	4	3	2	1
127	*	9	8	7	4	6	5	1	3	2
128	*	9	8	7	4	6	5	2	1	3
129	*	9	8	7	4	6	5	3	2	1
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131	*	9	8	7	5	4	6	2	1	3
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162	*	6	5	4	3	2	1	9	8	7

SYMMETRY ELEMENTS OF P GROUP OF BENZENE DIMER - Table V

NO	PI OPERATION											
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244	12	11	10	9	8	7	4	5	6	1	2	3
245	12	11	10	9	8	7	5	6	1	2	3	4

246	12	11	10	9	8	7	6	1	2	3	4	5
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248	12	11	10	9	8	7	4	3	2	1	6	5
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254	7	9	8	10	12	11	2	3	4	5	6	1
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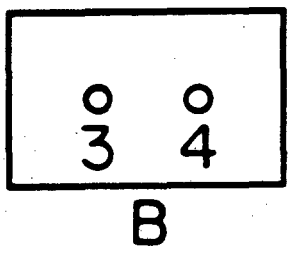
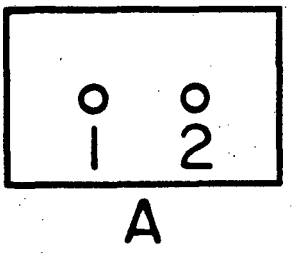
288	11	10	9	8	7	12	5	4	3	2	1	6

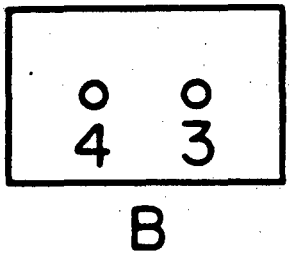
Figure Caption

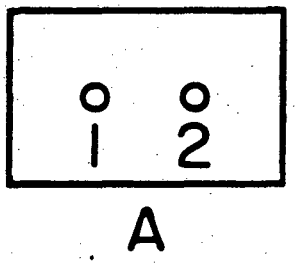
Figure 1. Particle-in-box model for hydrazine. The permutation group of the non-rigid molecule is a wreath product of the permutation group of boxes (S_2) with the permutation group of particles in a box (S_2).





(AB)(13)(24)





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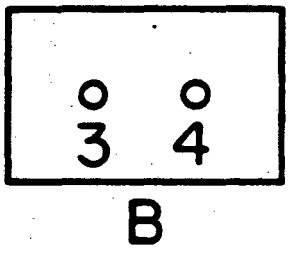

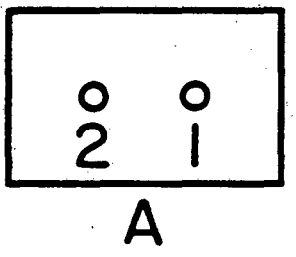

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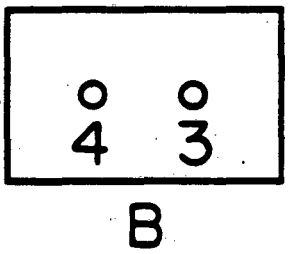

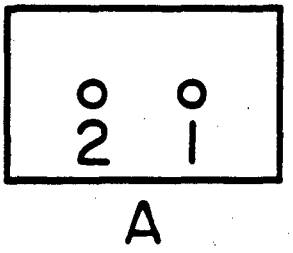

(AB) (14) (23)

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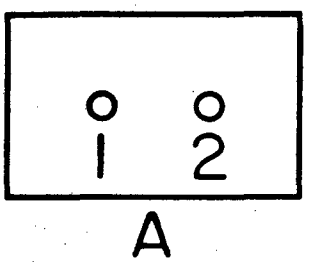
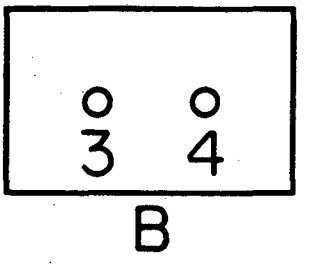
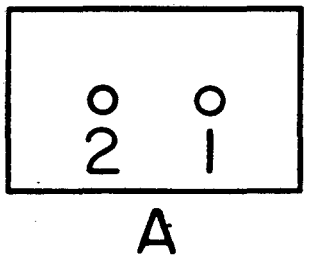
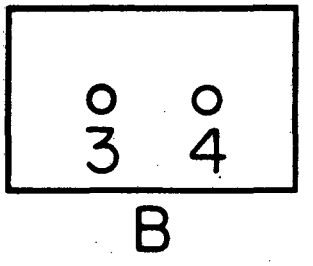




(A)(B)(1)(2)(3)(4)





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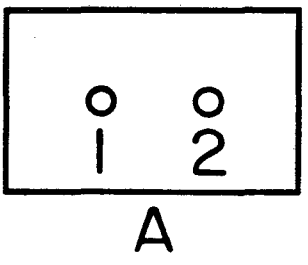

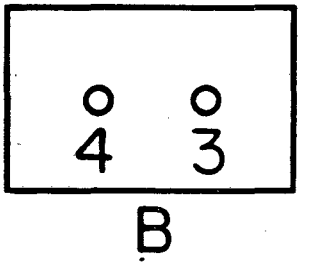

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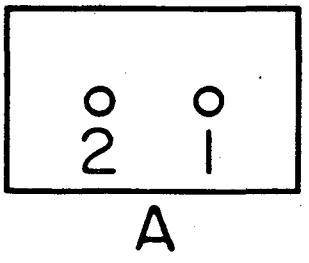

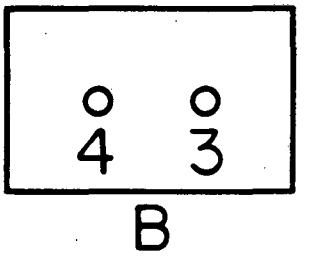

(A)(B)(12)(34)

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