The symmetry groups of nonrigid molecules as generalized wreath products and their representations

K. Balasubramanian

Citation: The Journal of Chemical Physics **72**, 665 (1980); doi: 10.1063/1.438963
View online: http://dx.doi.org/10.1063/1.438963
View Table of Contents: http://scitation.aip.org/content/aip/journal/jcp/72/1?ver=pdfcov
Published by the AIP Publishing

The symmetry groups of nonrigid molecules as generalized wreath products and their representations

K. Balasubramanian

Department of Chemistry, The Johns Hopkins University, Baltimore, Maryland 21218
(Received 28 December 1978; accepted 6 April 1979)

The symmetry groups of nonrigid molecules first defined by Longuet-Higgins, in the most general cases are generalized wreath product groups. We first outline the representation theory of wreath product groups. Then the representation theory of generalized wreath product groups is developed. Several illustrative examples of NMR groups are offered. The character tables of several nonrigid molecular groups are presented. An example of a nonrigid triphenyl molecule is given to illustrate the use of the generalized wreath product in deriving optical selection rules.

INTRODUCTION

Longuet-Higgins[1] defined a molecule to be nonrigid if it is in an electronic state that has several potential minima separated by surmountable energy barriers. The permutation group that includes only the permutations of the rigid nuclear framework of such nonrigid molecules is insufficient for interpreting many chemical and physical data obtained from their spectra, etc. For example, the microwave spectrum of the nonrigid hydrazine molecule needs to be interpreted by a group of higher order than its rigid molecular group. Kasuya,[2] in fact, interpreted the microwave spectrum of the nonrigid hydrazine molecule using a group of order 8. This group of order 8 is indeed the wreath product of S_2 with S_2. (S_2 denotes the symmetric group consisting of 2! elements). Woodman[3,4] defined the NMR group of a molecule and showed that groups of certain nonrigid molecules can be represented as semidirect products. The NMR groups in general cases are the generalized wreath product groups of the generalized composition of the NMR graph as we will show in a subsequent publication.[5] Serre[6-8] obtained the character tables of certain nonrigid molecules using the Mackey's theorems. The wreath product group is a particular form of the semidirect product. Considerable progress has been made inthe representation theory of the wreath product group.[9,10]

Certain characteristics pertaining to wreath product groups are not observed in all semidirect product groups. For example, the conjugacy classes of the wreath products of symmetric groups with other groups can be obtained by an elegant partition technique analogous to the method of obtaining the conjugacy classes of symmetric groups. Stone[11] obtained the character tables of the groups of nonrigid molecules containing methyl groups. However, this requires a knowledge of basis functions. Several other authors also worked in this area.[12] The present author[13] showed in the context of isomer enumeration that the permutation groups of nonrigid molecules, in general, are generalized wreath product groups. The symmetry groups of nonrigid molecules have several applications in spectroscopy,[1-5,8] certain problems of chemical reactivity,[14] and nuclear spin statistics.[15] The nonrigid molecular groups have applications in certain enumeration and combinatorial problems in chemistry.[13,16] The groups of nonrigid molecules are also useful in symmetry aspects in the investigation of scalar properties of molecules with internal rotation.[17] For these reasons, we undertake the study of the representation theory of the generalized wreath product groups. One of the objects of this investigation is to exploit certain special characteristics of wreath product groups and develop the representation theory of generalized wreath product groups. In Sec. II, we outline the representation theory of wreath product groups. In Sec. III, we develop the representation theory of generalized wreath product groups. In Sec. IV, we give certain applications.

II. WREATH PRODUCT GROUPS

A. Preliminaries

We start with the definition of wreath product groups. Let G be a permutation group acting on the set $\Omega = \{1, 2, \ldots, n\}$. Let H be another permutation group. The set

$$\{(g;\pi) \mid \pi \text{ mapping } \Omega \text{ into } H,\ g \in G\}$$

with the composition law

$$(g;\pi)(g';\pi') = (gg';\pi\pi'_g)$$

is called the wreath product of G with H and it is denoted as $G[H]$. In the above definition, π_g is the mapping π_g: $\Omega \to H$, defined by

$$\pi_g(i) = \pi(g^{-1}i)\ ,\quad \forall i \in \Omega\ ;$$

for two maps $\pi, \pi' : \Omega \to H$,

$$\pi\pi'(i) = \pi(i)\pi'(i)\ ,\quad \forall i \in \Omega\ .$$

Note that the notation that we follow is different from Kerber's notation. The set thus defined above forms a group. The identity is $(e;e')$, where e is the identity of G and e' is defined by

$$e'(i) = {}^1H\ ,\quad \forall i \in \Omega\ ,$$

where ${}^1H$ is the identity of the group H. The inverse of a typical element $(g;\pi)$ is $(g^{-1};\pi^{-1}_{g^{-1}})$. The associativity is verified as follows: Consider any three elements $(g_1;\pi^1)$, $(g_2;\pi^2)$, and $(g_3;\pi^3)$ in $G[H]$. Then,

$$[(g_1;\pi^1)(g_2;\pi^2)](g_3;\pi^3)$$
$$= (g_1g_2;\pi^1\pi^2_{g_1})(g_3;\pi^3) = (g_1g_2g_3;(\pi^1\pi^2_{g_1})\pi^3_{g_1g_2})\ .$$

However,

$$\pi^1\pi^2_{g_1}\pi^3_{g_1g_2}(i) = \pi^1(i)\pi^2(g_1^{-1}i)\pi^3(g_2^{-1}g_1^{-1}i)\ ,\quad i \in \Omega\ ; \tag{1}$$

consider

$$(g_1;\pi^1)[(g_2;\pi^2)(g_3;\pi^3)]$$
$$=(g_1;\pi^1)(g_2g_3;\pi^2\pi^3_{g_2})=[g_1g_2g_3;\pi^1(\pi^2\pi^3_{g_2})_{g_1}] .$$

By definition,

$$\pi^1(\pi^2\pi^3_{g_2})_{g_1}(i)=\pi^1(i)(\pi^2\pi^3_{g_2})(g_1^{-1}i)$$
$$=\pi^1(i)\pi^2(g_1^{-1}i)\pi^3(g_2^{-1}g_1^{-1}i) . \quad (2)$$

Since Eqs. (1) and (2) are identical, we have the associative law of multiplication of the elements of $G[H]$. Combinatorial books adopt an alternative notation for the elements of the wreath product groups. Every element of the wreath product in this notation is determined by an ordered pair of the form

$$(g;h_1, h_2, \ldots, h_n) ,$$

where $g\in G$ and $h_i \in H$. The order of the wreath product $G[H]$ is $|G|\,|H|^n$. To illustrate, consider a nonrigid molecule, namely, ethane. The group of permutations must include the point group operations and the permutations induced by internal rotations. Let the carbon atoms bear the labels 1 and 2. Then the set Ω is $\{1, 2\}$. With each carbon atom, there is an associated methyl rotor executing internal rotation. The group that characterizes each such internal rotor is C_3. Thus, each element of Ω can be assigned the group C_3. Let G be the point group acting on the two carbon atoms. Note that G contains both rotations and planes of symmetry. G can be seen to be C_{2v}. Hence, the point group of the nonrigid ethane molecule is the wreath product $C_{2v}[C_3]$. Any permutation of the nonrigid ethane molecule can be represented as $(g;h_1, h_2)$, $g\in C_{2v}$, $h_1 \in C_3$, and $h_2 \in C_3$.

B. A permutation representation of wreath product groups

Let H^* stand for the direct product of n copies of H, i.e.,

$$H^*=H_1\times H_2\times\cdots\times H_n ,$$

where

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

e is the identity of the group G, and ${}^1H$ is the identity of the group H. Let G' be the group

$$G'=\{(g;e')\,|\,g\in G\} .$$

Note that G' is isomorphic to G. However, G' acts on the whole molecular structure, whereas G acts only on Ω. A permutation representation of the wreath product of two groups [G acting on $\Omega=\{1, 2, \ldots, n\}$, and H acting on $\Gamma=\{1, 2, \ldots, m\}$] can be obtained first by dividing the set $\Delta=\{1, 2, 3, \ldots, mn\}$ into disjoint subsets $\Delta_1=\Gamma$, $\Delta_2, \ldots, \Delta_n$. Then the direct product of the groups H_i acting on Δ_i is formed and G' is "multiplied" with the group thus formed. In symbols,

$$G[H]=(H_1\times H_2\times\cdots\times H_n)G' .$$

Thus, $(H_1\times H_2\times\cdots\times H_n)G'$ is a permutation representation of the wreath product group $G[H]$. Note that H^* is an invariant subgroup of $G[H]$. Therefore, the group product H^*G' is a semidirect product. The fact that the groups of certain nonrigid molecules containing one type of internal rotor could be expressed as semidirect products was first noted by Altmann.[12(b)] Nevertheless, both Altmann and Serre[6-8] did not realize that these are wreath product groups which are special types of semidirect products.

Let us now illustrate the preceding discussion with the nonrigid ethane molecule. As shown earlier, the symmetry group of the nonrigid ethane molecule is $C_{2v}[C_3]$. The group G', which is isomorphic to C_{2v}, acting on the rigid framework is

$$G'=\{(1)(2)(3)(4)(5)(6),\ (14)(25)(36),\ (14)(26)(35)^*,\ (23)(56)^*\} ,$$

where 1, 2, 3 are the labels assigned to the hydrogen nuclei of one methyl rotor, while 4, 5, 6 are the labels of the hydrogen nuclei of the other methyl rotor. The groups H_1 and H_2 are given as follows:

$$H_1=\{(1)(2)(3),\ (123),\ (132)\} ,$$

$$H_2=\{(4)(5)(6),\ (456),\ (465)\} .$$

Therefore, a permutation representation of the wreath product $C_{2v}[C_3]$ is

$$\{[(1)(2)(3),\ (132),\ (123)]\times[(4)(5)(6),\ (456),\ (465)]\}$$
$$\circ\ \{(1)(2)(3)(4)(5)(6),\ (14)(25)(36),\ (14)(26)(35)^*,\ (23)(56)^*\}.$$

When one carries out the multiplication of the constituting permutations, one obtains the following set of 36 permutations:

$$\{(1)(2)(3)(4)(5)(6),\ (123),\ (132),\ (456),\ (465),\ (123)(456),$$
$$(123)(465),\ (132)(456),\ (132)(465),\ (14)(26)(35)^*,$$
$$(142635)^*,\ (143526)^*,\ (153624)^*,\ (162534)^*,\ (15)(24)(36)^*,$$
$$(163425)^*,\ (152436)^*,\ (16)(25)(34)^*,\ (14)(25)(36),\ (23)(56)^*,$$
$$(142536),\ (21)(56)^*,\ (143625),\ (13)(56)^*,\ (152634),$$
$$(23)(45)^*,\ (163524),\ (23)(64)^*,\ (153426),\ (12)(45)^*,$$
$$(16)(24)(35),\ (12)(46)^*,\ (15)(26)(34),\ (13)(45)^*,\ (162435),$$
$$(13)(46)^*\} .$$

Fortunately, this group happens to be the direct product $D_3\times D_3$ and hence the character table can be easily obtained.[1] The order of the groups of nonrigid molecules increases as $|H|^{|\Omega|}$ so that, unless there is a general theory for obtaining their irreducible representations, it is very difficult to obtain their character tables.

C. The wreath product of symmetric groups

The wreath products of symmetric groups are useful in obtaining the NMR groups defined by Woodman.[3,4] Hence, we devote this section to the wreath products of symmetric groups.

Let $S_n[H]$ be the group under consideration (S_n denotes the symmetric group containing $n!$ permutations). Let $(g;\pi)$ be an element of $S_n[H]$. If we adopt the convention to begin each cyclic factor with the least symbol included in the cycle decomposition of g, then we can associate with each cyclic factor $[j;g(j), g^2(j), \ldots, g^r(j)]$ of g the unique element

$$\pi\pi_g\pi_{g^2}\cdots\pi_{g^r}(j)=\pi(j)\pi[g^{-1}(j)]\cdots\pi[g^{-r}(j)]$$

in G. Let us call this element the cycle product associated with $[j;g(j),g^2(j),\ldots,g^r(j)]$ with respect to π. Let the permutation $g\in S_n$ be of the type $T_g=(a_1,a_2,\ldots,a_n)$ (denotes a_1 cycles of length 1, a_2 cycles of length 2, ..., a_n cycles of length n). There are a_k cycle products (defined above) associated with the a_k cycles of length k of g with respect to π. Let $C_1,C_2,\ldots,C_s$ be the conjugacy classes of H. If exactly a_{ik} of these cycle products belong to C_i, then the $s\times n$ matrix defined below is the cycle type of an element $(g;\pi)$ of the wreath product

$$T(g;\pi)=a_{ik}(1\le i\le s,\ 1\le k\le n)\ .$$

Let $P(m)$ denote the number of partitions of the integer m, with the convention that $P(0)=1$. Let n be partitioned into the ordered s-tuples $(n)=(n_1,n_2,\ldots,n_s)$ such that $\sum_i n_i=n$. (Recall that s is the number of conjugacy classes of H.) Then the number of conjugacy classes of $S_n[H]$ is

$$\sum_{(n)}P(n_1)P(n_2)\cdots P(n_s)\ .$$

For a proof, see Kerber.[9] The order of the conjugacy class whose matrix type is (a_{ik})[18] is given by

$$\frac{|S_n[H]|}{\prod_{i,k}a_{ik}!(k\cdot|H|/|C_i|)^{a_{ik}}}\ . \tag{3}$$

An explicit generating function for the conjugacy classes of $S_n[H]$ is derived in the Appendix.

As an example, for the conjugacy classes of the NMR group of borontrimethyl, the NMR group of $B(CH_3)_3$ can be seen to be $S_3[S_3]$.[5] Since the group S_3 has three classes, first find the ordered partitions of 3 into three parts. They are

$$(3,0,0),\ (0,3,0),\ (0,0,3),\ (2,1,0),\ (1,2,0),$$
$$(0,1,2),\ (0,2,1),\ (1,0,2),\ (2,0,1),\ (1,1,1)\ .$$

Thus,

$$\sum_{(n)}P(n_1)P(n_2)P(n_3)\ ,$$

where the summation is taken over all the ten triples, can be seen to be

$$3+3+3+2+2+2+2+2+2+1=22\ .$$

Hence, there are 22 classes in the group $S_3[S_3]$. The order of this group is $6\times6^3=1296$. The 22 matrices formed for the cycle types are shown in Table I. The order of each class is found using the formula (3). To illustrate, consider the eighteenth class in Table I. The matrix of the cycle type is

$$\begin{bmatrix}0&0&0\\0&0&0\\1&1&0\end{bmatrix}.$$

TABLE I. The conjugacy classes of the NMR group of boron trimethyl. The matrices are the cycle types. The order of each class is found using the formula (3) (see text).

No.	Class representative	Matrix of the cycle type	Order
(1)	{1; (123), (123), (123)} (123) (456) (789)	$\begin{bmatrix}0&0&0\\0&0&0\\3&0&0\end{bmatrix}$	8
(2)	{1; (12), (12), (12)} (12) (45) (78)	$\begin{bmatrix}0&0&0\\3&0&0\\0&0&0\end{bmatrix}$	27
(3)	{1; 1, 1, 1} 1	$\begin{bmatrix}3&0&0\\0&0&0\\0&0&0\end{bmatrix}$	1
(4)	{1; (12), 1, 1} (12)	$\begin{bmatrix}2&0&0\\1&0&0\\0&0&0\end{bmatrix}$	9
(5)	{1; (12), (12), (123)} (12) (45) (789)	$\begin{bmatrix}0&0&0\\2&0&0\\1&0&0\end{bmatrix}$	54
(6)	{1; 1, (123), (123)} (456) (789)	$\begin{bmatrix}1&0&0\\0&0&0\\2&0&0\end{bmatrix}$	12
(7)	{1; (12), (123), (123)} (12) (456) (789)	$\begin{bmatrix}0&0&0\\1&0&0\\2&0&0\end{bmatrix}$	36
(8)	{1; 1, (12), (12)} (12)(45)	$\begin{bmatrix}1&0&0\\2&0&0\\0&0&0\end{bmatrix}$	27
(9)	{1; 1, 1, (123)} (789)	$\begin{bmatrix}2&0&0\\0&0&0\\1&0&0\end{bmatrix}$	6
(10)	{1; 1, (12), (123)} (45) (789)	$\begin{bmatrix}1&0&0\\1&0&0\\1&0&0\end{bmatrix}$	36
(11)	{(123); 1, 1, 1} (147) (268) (359)	$\begin{bmatrix}0&0&1\\0&0&0\\0&0&0\end{bmatrix}$	72
(12)	{(123); (12), 1, 1} (168247) (359)	$\begin{bmatrix}0&0&0\\0&0&1\\0&0&0\end{bmatrix}$	216
(13)	{(123); (123), (123), (123)} (167258349)	$\begin{bmatrix}0&0&0\\0&0&0\\0&0&1\end{bmatrix}$	144
(14)	{(12); 1, 1, 1} (14) (35) (26)	$\begin{bmatrix}1&1&0\\0&0&0\\0&0&0\end{bmatrix}$	18
(15)	{(12); (123), 1,1} (162534)	$\begin{bmatrix}1&0&0\\0&0&0\\0&1&0\end{bmatrix}$	36
(16)	{(12); (12), 1, 1} (1624) (35)	$\begin{bmatrix}1&0&0\\0&1&0\\0&0&0\end{bmatrix}$	54
(17)	{(12); (123), (123), (123)} (16) (25) (34) (789)	$\begin{bmatrix}0&1&0\\0&0&0\\1&0&0\end{bmatrix}$	36
(18)	{(12); (12), (12), (123)} (162435) (789)	$\begin{bmatrix}0&0&0\\0&0&0\\1&1&0\end{bmatrix}$	72

TABLE I (*Continued*)

No.	Class representative	Matrix of the cycle type	Order
(19)	{(12); (12), 1, (123)} (1624) (35) (789)	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$	108
(20)	{(12); (123), (123), (12)} (16) (25) (34) (78)	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	54
(21)	{(12); 1, (123), (12)} (143526) (78)	$\begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$	108
(22)	{(12); (123), (12), (12)} (1625) (34) (78)	$\begin{bmatrix} 0 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	162

The order of this class is

$$\frac{1296}{1!\,(1\cdot\frac{6}{2})^1\cdot 1!\,(2\cdot\frac{6}{2})^1}=72\ .$$

To obtain the cycle decomposition of a representative in a conjugacy class, we use the permutation representation described earlier. By way of illustration, consider the class 13, viz., {(123); (123), (123), (123)}. The permutation representation of this class is

$$[(123)\times(456)\times(789)]\ (147)(268)(359)=(167258349)\ .$$

D. Representations of wreath products

Since wreath products are particular types of semidirect products, we may obtain their irreducible representations using Mackey's theory of the semidirect product.[19] Nevertheless, certain particular features of wreath product groups which are not found in all semidirect products enable certain simplifications. The procedure outlined by Kerber[9,10(a)] seems to be of particular importance to wreath product groups. We present the same here.

Recall that $H^*=H_1\times H_2\times\cdots\times H_n$, with $H\approx H_i=\{(e;\pi)\,|\,\pi:\Omega\to H/\pi(j)={}^1H\in H,\ \forall j\neq i\}$. Since H^* is a direct product of the groups $H_1, H_2, \ldots, H_n$, the irreducible presentations of H^* are the outer tensor products

$$F^*=F_1\#F_2\#F_3\#\cdots\#F_n\ ,$$

where # denotes the outer tensor product. Formal definitions of outer and inner tensor products can be found in Curtis and Reiner.[19] However, in simple terms, the matrices of outer tensor products can be obtained as the Kronecker products. Symbolically,

$$F^*(e,\pi)=F_1[\Pi(1)]\times F_2[\Pi(2)]\times\cdots\times F_n[\Pi(n)]$$
$$=f_{i_1k_1}[\Pi(1)]f_{i_2k_2}[\Pi(2)]\cdots f_{i_nk_n}[\Pi(n)]\quad ,$$

if $F(h)=f_{ik}(h)$ for $h\in H$. To obtain the irreducible representations of wreath product groups, first we determine the inertia group $G_{F^*}[H]$, which is defined as

$$G_{F^*}[H]=\{(g;\pi)\,|\,F^{*(g;\pi)}\sim F^*\}\ ,$$

where

$$F^{*(g;\pi)}(e;\pi')=F^*(g;\pi)^{-1}(e;\pi')(g;\pi)\ (\sim \text{denotes equivalency}).$$

The group $G_{F^*}[H]$ by definition is the product $H^*G'_{F^*}$; G'_{F^*} is called the inertia factor of F^* and

$$G'_{F^*}=\{(g;e')\,|\,F^{*(g;e')}\sim F^*\}\ .$$

Let $F^1, F^2, \ldots, F^\gamma$ be a fixed arrangement of γ pairwise nonequivalent representations of H. F^* is said to be of the type $(n)=(n_1, n_2, \ldots, n_\gamma)$ with respect to the above arrangement if n_j is the number of factors F_i of F^* equivalent of F^j. Let S_{n_j} be the subgroup of S_n consisting of the elements permuting exactly the n_j indices of the n_j factors F_i of F^* which are equivalent to F^j. Define $S'_{(n)}$ to be $S'_{n_1}\times S'_{n_2}\cdots\times S'_{n_\gamma}$ with

$$S'_{n_j}=\{(g;e')\,|\,g\in S_{n_j}\}\ .$$

In this setup, Kerber[9] proved that

$$G'_{F^*}=G'\cap S_{(n)}\ .$$

The representations $\tilde{F}^*$ whose matrices are defined as follows form the representations of $G_{F^*}[H]$:

$$\tilde{F}^*(g;\pi)=f_{i_1k_{g^{-1}(1)}}[\Pi(1)]f_{i_2k_{g^{-1}(2)}}[\Pi(2)]\cdots f_{i_nk_{g^{-1}(n)}}[\Pi(n)]\ .$$

Alternatively, $\tilde{F}^*(g;\pi)$ is found from $F^*(e;\pi)$ by a suitable permutation of the columns of $F^*(e;\pi)$ which is determined by the operation g^{-1} acting on the second index.

Before we proceed to consider the irreducible representations of the wreath product group $G[H]$, we need to know the concept of induced representations. Let G be a group and K be its normal subgroup. Since K is a normal subgroup, the quotient group G/K is well defined. It is possible to construct the irreducible representations of G from the irreducible representations of K. Let Γ be an irreducible representation of K. Then an irreducible representation of G induced by Γ, denoted as $\Gamma\uparrow G$, is constructed using the following results:

(i) The dimension of $\Gamma\uparrow G$ is

$$\dim(\Gamma)\,|G|/|K|\ .$$

(ii) Let $\sigma\in G/K$ be the coset of the form $\sigma=KS_\sigma$, with $S_\sigma\in G$. Let $k\to\psi(k)$ be the character of the representation Γ. Then the character $g\to\chi(g)$ induced by Γ is given by

$$\chi(g)=\sum_\sigma \psi(S_\sigma g S_\sigma^{-1})\ ,$$

where the summation is taken over all $\sigma\in G/K$ for which $\sigma g=\sigma$. For a proof and an expository survey on induced representation, see Coleman[20] or Curtis and Reiner.[19]

Let F' be an irreducible representation of the inertia factor G'. Let $\tilde{F}^*$ be determined using the method outlined above. Then the representations induced by the irreducible representations obtained by multiplying $\tilde{F}^*$ and F' are the irreducible representations of the wreath product of G with H. In Kerber's notation,

$$(\tilde{F}^*\otimes F')\uparrow G[H]$$

are the irreducible representations of $G[H]$.

Note that, since the representation $(\tilde{F}^* \otimes F') \uparrow G[H]$ is the induced representation of $\tilde{F}^* \otimes F'$ over $G[H]$, the dimension of $(\tilde{F}^* \otimes F') \uparrow G[H]$ is

$$\dim[(\tilde{F}^* \otimes F') \uparrow G[H]] = \dim(\tilde{F}^* \otimes F') \frac{|G[H]|}{|G_{F^*}[H]|}.$$

In particular, if $G_{F^*}[H] = G[H]$, then $(\tilde{F}^* \otimes F') \uparrow G[H] = \tilde{F}^* \oplus F'$.

The representation matrices of the representations of H can be elegantly obtained if H happens to be S_m for some m. In this case, to obtain F^*, first one needs to know F. From the partition associated with F, the dimension of F is determined by the Frame-Robinson-Thrall's theorem.[21] The representation matrix is obtained using the representation theory of symmetric groups which can be found elsewhere.[22] In this case, a representation F will be denoted by $[P(m)]$, where $P(m)$ is the partition associated with F. The columns of $[P(m)](h)$, $h \in H$, will be labeled by the Young tableaux[22] associated with $P(m)$. F^* is the n-fold outer tensor product of copies of F.

Now, we shall illustrate the construction of $\tilde{F}^*$ with a simple example since this deserves attention. Let us find the matrix of the representation $[2,1]\#[2,1]$ $[(12);e']$ where $[2,1]$ is the irreducible representation corresponding to the partition $(2,1)$ in S_3:

$$[2,1]\#[2,1](e;e') = \begin{array}{cc} \genfrac{}{}{0pt}{}{12}{3} & \genfrac{}{}{0pt}{}{13}{2} \\ \multicolumn{2}{c}{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}} \end{array} \begin{array}{cc} \genfrac{}{}{0pt}{}{45}{6} & \genfrac{}{}{0pt}{}{46}{5} \\ \multicolumn{2}{c}{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}} \end{array}$$

$$= \begin{array}{cccc} \genfrac{}{}{0pt}{}{12\,45}{3\;\,6} & \genfrac{}{}{0pt}{}{12\,46}{3\;\,5} & \genfrac{}{}{0pt}{}{13\,45}{2\;\,6} & \genfrac{}{}{0pt}{}{13\,46}{2\;\,5} \\ \multicolumn{4}{c}{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}} \end{array},$$

which is of the form $f^1_{i_1k_1}(1)\, f^2_{i_2k_2}(1)$:

$$\widetilde{[2,1]\#[2,1]}\,[(12);e'] = f^1_{i_1k_{(12)^{-1}(1)}}(1)\, f^2_{i_2k_{(12)^{-1}(2)}}(1)$$

$$= f^1_{i_1k_2}(1)\, f^2_{i_2k_1}(1)$$

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

Note that each column of $[2,1]\#[2,1]\,(e;e')$ is determined by a pair of Young tableaus. The columns of $\widetilde{[2,1]\#[2,1]}\,[(12);e']$ are determined by the action of g^{-1} on Young tableaus, shown below. Let $T_1(1) = \genfrac{}{}{0pt}{}{12}{3}$, $T_2(1) = \genfrac{}{}{0pt}{}{13}{2}$, $T_1(2) = \genfrac{}{}{0pt}{}{45}{6}$, and $T_2(2) = \genfrac{}{}{0pt}{}{46}{5}$. In general, if $T_l(i)$ is a Young tableau associated with the partition $p(m)$ which labels a column of $F_i(h)$, $h \in H$, then

$$g^{-1}T_l(i) = T_l(g^{-1}i).$$

In this example, since $g = (12)$,

$$g^{-1}T_1(1) = T_1(2),$$

$$g^{-1}T_2(1) = T_2(2),$$

$$g^{-1}T_1(2) = T_1(1),$$

$$g^{-1}T_2(2) = T_2(1).$$

Thus, the columns of $\widetilde{[2,1]\#[2,1]}\,[(12);e']$ are determined by the pairs $\genfrac{}{}{0pt}{}{45}{6}\genfrac{}{}{0pt}{}{12}{3}$, $\genfrac{}{}{0pt}{}{45}{6}\genfrac{}{}{0pt}{}{13}{2}$, $\genfrac{}{}{0pt}{}{46}{5}\genfrac{}{}{0pt}{}{12}{3}$, and $\genfrac{}{}{0pt}{}{46}{5}\genfrac{}{}{0pt}{}{13}{2}$. This is precisely the permutation $(1)(23)(4)$ of the four columns of $[2,1]\#[2,1](e;e')$. Alternatively, if C_{ji} is the jth column in the ith representation, then a column of the n-fold outer tensor product $F^*(e;\pi)$ is determined by an unordered n-tuple $(C_{j_11}, C_{j_22}, \ldots, C_{j_nn})$. The corresponding column of $\tilde{F}^*(g;\pi)$ is determined by the action of g^{-1} on this unordered n-tuple as shown below:

$$g^1(C_{j_11}, C_{j_22}, \ldots, C_{j_nn}) = (C_{j_{1g^{-1}}1}, C_{j_{2g^{-1}}2}, \ldots, C_{j_{ng^{-1}}n}).$$

Let us illustrate the construction of the character table of wreath product groups with the simplest example, namely $S_2[S_2]$. $S_2[S_2]$ is the rotational subgroup of the nonrigid hydrazine molecule. Let the representations of the group S_2 be denoted as $[1^2]$ and $[2]$, $[2]$ being the identity representation. Then the representations of the basis group S_2^* are

$$[2]\#[2], [2]\#[1^2], [1^2]\#[2], [1^2]\#[1^2].$$

The pairwise different types of S_2^* are

$$[2]\#[2], [2]\#[1^2], [1^2]\#[1^2].$$

The corresponding inertia groups are $S_2[S_2]$, $S_2 \times S_2$, and $S_2[S_2]$, respectively. Hence, the inertia factors are S_2', S_1', and S_2', respectively. Consequently, the irreducible representations of $S_2[S_2]$ are

$$\widetilde{[2]\#[2]} \otimes [2]' = \widetilde{[2]\#[2]},$$

$$\widetilde{[2]\#[2]} \otimes [1^2]',$$

$$\widetilde{[2]\#[1^2]} \otimes [1]' \uparrow S_2[S_2] = [2]\#[1^2] \uparrow S_2[S_2],$$

$$\widetilde{[1^2]\#[1^2]} \otimes [2]' = \widetilde{[1^2]\#[1^2]},$$

$$\widetilde{[1^2]\#[1^2]} \otimes [1^2]'.$$

These are the five irreducible representations of dimensions 1, 1, 2, 1, and 1, respectively, satisfying the rule

$$4 \cdot 1^2 + 1 \cdot 2^2 = |S_2[S_2]| = 8.$$

The character table of $S_2[S_2]$ is shown in Table II. The first representation of $S_2[S_2]$ is the identity representation. The second representation is obtained by multiplying the first representation with $[1^2]'$. From the character table of S_2, it can be seen that $[1^2]'$ has the character 1 in all classes where g is the identity and -1 in all the classes where g is (12). Thus, when we

TABLE II. The character table of the wreath product $S_2[S_2]$, the rotational subgroup of the nonrigid hydrazine molecule.

Conjugacy class / order	$\{1;\ 1\ 1\}$ 1	$\{1;\ (12),\ 1\}$ (12)	$\{1;\ (12),\ (12)\}$ (12) (34)	$\{(12);\ 1,\ 1\}$ (14) (23)	$\{(12);\ (12),\ 1\}$ (1324)
order	1	2	1	2	2
$\widetilde{[2]\#[2]}\otimes[2]'$	1	1	1	1	1
$\widetilde{[2]\#[2]}\otimes[1^2]'$	1	1	1	-1	-1
$[2]\#[1^2]\uparrow S_2[S_2]$	2	0	-2	0	0
$\widetilde{[1^2]\#[1^2]}\otimes[2]'$	1	-1	1	$+1$	-1
$\widetilde{[1^2]\#[1^2]}\otimes[1^2]'$	1	-1	1	-1	$+1$

multiply $[1^2]'$ with $\widetilde{[2]\#[2]}$, we obtain the second representation of $S_2[S_2]$. The third representation in Table II is obtained by inducing the representation $[2]\#[1^2]$ over the whole group $S_2[S_2]$. The fourth representation is easily determined. The last representation is the multiplication of the fourth and $[1^2]'$. The conjugacy classes, the order of each class, and the representative of each class can be obtained using the method outlined earlier.

This is a detailed description of the rotational subgroup of the nonrigid hydrazine molecule. The character table of the whole point group was obtained first by Longuet-Higgins.[1] The character table of the whole group can be obtained easily from $S_2[S_2]$. Kerber[9] worked out the character table of $S_2[S_3]$. Several other authors[3,8] also worked out the character table of the group $S_2[S_3]$, the NMR group of ethane. Table III[23] shows the character table of $S_3[S_3]$, the NMR group of $B(CH_3)_3$ and isobutane. The conjugacy classes and the order of each conjugacy class of the group $S_3[S_3]$ have already been determined in Table I.

III. GENERALIZED WREATH PRODUCT GROUPS

Let $\Omega=\{1, 2, \ldots, n\}$ be partitioned into the mutually disjoint sets $Y_1, Y_2, \ldots, Y_t$. Let $H_1, H_2, \ldots, H_t$ be t permutation groups. Let π_i be a map from Y_i to H_i $(i=1, 2, \ldots, t)$. Then the set $\{(g;\pi_1, \pi_2, \ldots, \pi_t)\,|\,g\in G, \pi_i: Y_i \to H_i\}$ is called the generalized wreath product. Each element in the generalized wreath product can also be represented by an ordered $(t+1)$-tuple of the form $(g;h_{11}, h_{12}, \ldots, h_{1m_1};h_{21}, h_{22}, \ldots, h_{2m_2};\ldots;h_{t1}, h_{t2}, \ldots, h_{tm_t})$, where $m_i=|Y_i|$, $g\in G$, and $h_{ij}\in H_i$. It can be seen that the generalized wreath product set forms a group and it is denoted as $G[H_1, H_2, \ldots, H_t]$.

To illustrate, consider the nonrigid propane molecule. The NMR group of this molecule which contains those permutations among magnetically equivalent nuclei preserving the NMR coupling constants is obtained as follows[5]: Let S_2 be the group acting on the three carbon atoms. The sets Ω, Y_1, and Y_2 are $\Omega=\{1, 2, 3\}$, $Y_1=\{1, 3\}$, and $Y_2=\{2\}$, respectively. Let H_1 be the group acting on the protons corresponding to the elements of the set Y_1. Let H_2 be the group acting on the protons corresponding to the set Y_2. H_1 is S_3 and H_2 is S_2. Thus, there are more than one type of H group acting on the protons. The NMR group of propane is the generalized wreath product $S_2[S_3, S_2]$.[5] Each element of the NMR group of propane can be represented as $(g;\pi_1, \pi_2)$, $g\in S_2$, π_1 mapping Y_1 to H_1, and π_2 mapping Y_2 to H_2. We may also represent it by a triple of the form $(g;h_{11}, h_{12};h_{21})$; $g\in G$; $h_{11}, h_{12}\in H_1=S_3$; and $h_{21}\in H_2=S_2$.

The author[13] has already shown in the context of isomer enumeration that every element $g\in G$ has all its orbits within the same Y set. Alternatively, any $g\in G$ permutes the elements of Ω such that any permutation has all the elements within a cycle, in the same Y set. Let g_i be the cycle product of $g\in G$ contained in the set Y_i. Then, to each $g\in G$, we can assign an unique ordered t-tuple $(g_1, g_2, \ldots, g_t)$ which is determined by its cycle decomposition. Let G_i be the set of all cycle products of the elements of G contained in the set Y_i. Then we have the following theorem:

Theorem (1): G_i forms a group.

Proof: since G is a group, for any two elements g and g' in G, $gg'\in G$. Let g and g' have cycle decompositions of the form $(g_1, g_2, \ldots, g_t)$ and $(g_1', g_2', \ldots, g_t')$, which are determined uniquely as described above. It can be seen that

$$gg'=(g_1g_1', g_2g_2', \ldots, g_tg_t')\,.$$

Since $gg'\in G$, $g_ig_i'\in G_i$. Thus, the closure property is satisfied in G_i. The identity of G has the unique decomposition $(e_1, e_2, \ldots, e_i, \ldots, e_t)$ which determines the identity $e_i\in G_i$. The inverse of an element $g\in G$ which has the form $(g_1^{-1}, g_2^{-2}, g_i^{-1}, \ldots, g_t^{-1})$ determines $g_i^{-1}\in G_i$ for every $g_i\in G_i$. Thus, G_i is a group.

The multiplication of two elements of the generalized wreath product in their "map representation" is defined as follows:

$$(g;\pi_1, \pi_2, \ldots, \pi_t)\cdot(g';\pi_1', \pi_2', \ldots, \pi_t')$$
$$=(gg';\pi_1\pi_{1g_1}', \pi_2\pi_{2g_2}', \ldots, \pi_t\pi_{tg_t}')\,,$$

where g_i is the cycle product of g contained in the set Y_i. π_{ig_i}' is defined by

$$\pi_{ig_i}'[g_i(j)]=\pi_i'(j)\,,\qquad j\in Y_i\,.$$

A permutation representation of the generalized wreath product group $G[H_1, H_2, \ldots, H_t]$ with G acting on $\Omega=\{1, 2, \ldots, n\}$ and H_i acting on $T_i=\{1, 2, \ldots, t_i\}$ can be obtained first by dividing the set $\Delta=\{1, 2, \ldots, n\prod_{i=1}^t t_i\}$ into disjoint subsets $\Delta_{11}, \Delta_{12}, \ldots, \Delta_{1m_1}, \Delta_{21}, \ldots, \Delta_{2m_2},$

TABLE III. The character table of $S_3[S_3]$, the NMR group of boron trimethyl.

	{1; 1, 1} 1	{1;(12), (12), (12)} (12) (45) (78)	{1; (123), (123), (123)} (123) (456) (789)	{1; (12), 1, 1} (12)	{1; (12), (12), (123)} (12) (45) (789)	{1; 1, (123), (123)} (456) (789)	{1; (12), (123), (123)} (12) (456) (789)	{1; (12), (12), 1} (12) (45)	{1; (123), 1, 1} (123)	{1; 1, (12), (123)} (45) (789)	{(123); 1, 1, 1} (147) (268) (359)	{(123); (12), 1, 1} (168247) (359)	{(123); (123), (123), (123)} (167258349)	{(12); 1, 1, 1} (14) (35) (26)	{(12); (123), 1, 1} (162534)	{(12); (12), 1, 1} (1624) (35)	{(12); (123), (123), (123)} (16) (25) (34) (789)	{(12); (12), (12) (123)} (162435) (789)	{(12); (12), 1, (123)} (1624) (35) (789)	{(12); (123), (123), (12)} (16) (25) (34) (78)	{(12); 1, (123), (12)} (143526) (78)	{(12); (123), (12), (12)} (1625) (34) (78)
Order	1	27	8	9	54	12	36	27	6	36	72	216	144	18	36	54	36	72	108	54	108	162
Γ_{1}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
Γ_{2}	1	−1	1	−1	1	1	−1	1	1	−1	1	−1	1	−1	1	1	−1	−1	1	1	1	−1
Γ_{3}	1	1	1	1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	−1
Γ_{4}	1	−1	1	−1	1	1	−1	1	1	−1	1	−1	1	1	1	−1	1	1	−1	−1	−1	1
Γ_{5}	2	2	2	2	2	1	2	2	2	2	−1	−1	−1	0	0	0	0	0	0	0	0	0
Γ_{6}	2	−2	2	−2	2	2	−2	2	2	−2	−1	1	−1	0	0	0	0	0	0	0	0	0
Γ_{7}	3	3	3	−1	−1	3	−1	−1	3	−1	0	0	0	−1	−1	1	−1	−1	1	−1	−1	1
Γ_{8}	3	−3	3	1	−1	3	1	−1	3	1	0	0	0	1	1	1	1	1	1	−1	−1	−1
Γ_{9}	3	3	3	−1	−1	3	−1	−1	3	−1	0	0	0	1	1	−1	1	1	−1	1	1	−1
Γ_{10}	3	−3	3	1	−1	3	1	−1	3	1	0	0	0	−1	−1	−1	−1	−1	−1	1	1	1
Γ_{11}	6	0	−3	4	−1	0	−2	2	3	1	0	0	0	2	2	2	−1	−1	−1	0	0	0
Γ_{12}	6	0	−3	−4	−1	0	2	2	3	−1	0	0	0	−2	−2	2	1	1	−1	0	0	0
Γ_{13}	6	0	−3	4	−1	0	−2	2	3	1	0	0	0	−2	−2	−2	1	1	1	0	0	0
Γ_{14}	6	0	−3	−4	−1	0	2	2	3	−1	0	0	0	2	2	−2	−1	−1	1	0	0	0
Γ_{15}	8	0	−1	0	0	2	0	0	−4	0	2	0	−1	−4	2	0	2	−1	0	0	0	0
Γ_{16}	8	0	−1	0	0	2	0	0	−4	0	2	0	−1	4	−2	0	−2	1	0	0	0	0
Γ_{17}	12	0	3	4	0	−3	1	0	0	−2	0	0	0	−2	1	0	−2	1	0	−2	1	0
Γ_{18}	12	0	3	−4	0	−3	−1	0	0	2	0	0	0	2	−1	0	2	−1	0	−2	1	0
Γ_{19}	12	0	3	4	0	−3	1	0	0	−2	0	0	0	2	−1	0	2	−1	0	2	−1	0
Γ_{20}	12	0	3	−4	0	−3	−1	0	0	2	0	0	0	−2	1	0	−2	1	0	2	−1	0
Γ_{21}	12	0	−6	0	2	0	0	−4	6	0	0	0	0	0	0	0	0	0	0	0	0	0
Γ_{22}	16	0	−2	0	0	4	0	0	−8	0	−2	0	1	0	0	0	0	0	0	0	0	0

$\ldots, \Delta_{t1}, \ldots, \Delta_{tm_t}$. Then, for a given i, the direct product of the groups H_{ij} acting on Δ_{ij} is obtained varying j from 1 to m_i. Subsequently, the permutational representation of the generalized wreath product is

$$G[H_1, H_2, \ldots, H_t] \approx [(H_{11} \times H_{12} \times \cdots \times H_{1m_1}) \times (H_{21} \times H_{22} \times \cdots \times H_{2m_2}) \times \cdots \times (H_{t1} \times H_{t2} \times \cdots \times H_{tm_t})] \cdot G' .$$

The direct product $(H_{11} \times H_{12} \times \cdots \times H_{1m_1}) \times (H_{21} \times H_{22} \times \cdots \times H_{2m_2}) \cdots (H_{t1} \times H_{t2} \times \cdots \times H_{tm_t})$, which is also denoted as $H_1^{m_1^*} \times H_2^{m_2^*} \times \cdots \times H_t^{m_t^*}$, is called the basis group of $G[H_1, H_2, \ldots, H_t]$. It can be seen that $H_1^{m_1^*} \times H_2^{m_2^*} \times \cdots \times H_t^{m_t^*}$ is an invariant subgroup of $G[H_1, H_2, \ldots, H_t]$. Therefore, the permutation representation obtained above is the semidirect product of $H_1^{m_1^*} \times H_2^{m_2^*} \times \cdots \times H_t^{m_t^*}$ with G'.

B. Representations of generalized wreath product groups

In this section, we develop a method for constructing the irreducible representations of $G[H_1, H_2, \ldots, H_t]$ from the irreducible representations of $G, H_1, H_2, \ldots, H_t$. It is interesting that the combinatorial theorem of Polya,[24] which was essentially developed for the enumeration of configurations under group actions and chemical isomers, finds an important application in finding the number of irreducible representations of $G[H_1, H_2, \ldots, H_t]$.

Let the irreducible representations of $H_1^{m_1^*} \times H_2^{m_2^*} \times \cdots \times H_t^{m_t^*}$ be denoted as $F_1^{m_1^*} \# F_2^{m_2^*} \# \cdots \# F_t^{m_t^*}$, where $F_i^{m_i^*}$ is the outer tensor product $F_{i1} \# F_{i2} \# \cdots \# F_{im_i}$; F_{ij} is an irreducible representation of H_i. The group G acts on $\{\#_i F_i^{m_i^*}\}$. Two irreducible representations $\#_i F_i^{m_i^*}$ and $\#_i F_i'^{m_i^*}$ in F, the set of all $\#_i F_i^{m_i^*}$, are said to be equivalent if there exists a $g \in G$, such that

$$g \mathop{\#}_i F_i^{m_i^*} = \mathop{\#}_i F_i'^{m_i^*} ,$$

where g acts on $\#_i F_i^{m_i^*}$ as follows: By theorem (1), a given $g \in G$ uniquely determines a g_i in the group G_i; g_i permutes the elements of the set Y_i. Define

$$g_i(F_{i1} \# F_{i2} \# \cdots \# F_{im_i}) = F_{ig_i(1)} \# F_{ig_i(2)} \# \cdots \# F_{ig_i(m_i)} .$$

Hence,

$$g\{(F_{11} \# F_{12} \# \cdots \# F_{1m_1}) \# (F_{21} \# F_{22} \# \cdots \# F_{2m_2}) \# \cdots \# (F_{t1} \# F_{t2} \# \cdots \# F_{tm_t})\}$$
$$= (F_{1g_1(1)} \# F_{1g_1(2)} \# \cdots \# F_{1g_1(m_1)}) \# (F_{2g_2(1)} \# F_{2g_2(2)} \# \cdots \# F_{2g_2(m_2)}) \# \cdots \# (F_{tg_t(1)} \# F_{tg_t(2)} \# \cdots \# F_{tg_t(m_t)}) .$$

Two representations that are equivalent belong to the same class. Thus, G divides F into equivalence classes The inertia group of each class of F and the corresponding inertia factors should be determined. Suppose F' is the inertia factor of $\#_i F_i^{m_i^*}$ in a class of F. Then irreducible representations of $G[H_1, H_2, \ldots, H_t]$ are the representations induced by $\widetilde{\#_i F_i^{m_i^*}} \otimes F'$. In symbols, $(\widetilde{\#_i F_i^{m_i^*}} \otimes F') \uparrow G[H_1, H_2, \ldots, H_t]$ are the irreducible representations of $G[H_1, H_2, \ldots, H_t]$.

Now, we give a method for finding the number of classes of F, the set of all irreducible representations of the basis group and the number of irreducible representations of $G[H_1, H_2, \ldots, H_t]$. The cycle index of a group G is defined as

$$P_G(S_1, S_2, \ldots) = \frac{1}{|G|} \sum_{g \in G} S_1^{b_1} S_2^{b_2} \cdots ,$$

where $S_1^{b_1} S_2^{b_2} \cdots$ is a representation of a typical permutation $g \in G$ having b_1 cycles of length 1, b_2 cycles of length 2, etc. Since G has all its cycles in the same Y set, the cycle index of G has a particular form. Let S_{ij} be a cycle of length j in the set Y_i. Let $C_{ij}(g)$ be the number of j cycles of $g \in G$ in the set Y_i. Then the cycle index of G is

$$P_G = \frac{1}{|G|} \sum_{g \in G} \prod_i \prod_j S_{ij}^{C_{ij}(g)} .$$

To each irreducible representation of H_i, let us assign a weight α_{ij}. Let the number of irreducible representations of H_i be n_i. Then the number of classes or irreducible representations of the basis group is

$$P_G(S_{ij} - n_i) . \tag{4}$$

It is obtained by replacing every cycle of length j in the set Y_i by n_i. The generating function for the classes of irreducible representations is

$$C = P_G\left(S_{ik} - \sum_j \alpha_{ij}^k\right) . \tag{5}$$

The coefficient of

$$\alpha_{11}^{b_{11}} \alpha_{12}^{b_{12}} \cdots \alpha_{tm_t}^{b_{tm_t}}$$

in Eq. (5) gives the number of classes of irreducible representations (of the basis group) of the form

$$(F_{11})^{b_{11}} (F_{12})^{b_{12}} \# \cdots \# (F_{tm_t})^{b_{tm_t}} .$$

As an example, for the irreducible representations of the NMR group of propane $S_2[S_3, S_2]$, let the irreducible representations of S_2 be denoted as $[2]$ and $[1^2]$. Let the irreducible representations of S_3 be $[3]$, $[2,1]$, and $[1^3]$. The basis group of $S_2[S_3, S_2]$ is therefore $(S_3 \times S_3) \times S_2$, where S_2 acts on the protons corresponding to the set Y_2, the first S_3 in $(S_3 \times S_3) \times S_2$ acts on the protons corresponding to the carbon atom 1, while the second S_3 acts on the protons corresponding to the carbon atom 3. The 18 irreducible representations of $(S_3 \times S_3) \times S_2$ are shown below. The suffixes below the irreducible representations show the carbon atoms whose protons are acted upon by the corresponding group to which the irreducible representations belong:

Γ_1: $([3]_1 \# [3]_3) \# [2]_2$,

Γ_2: $([3]_1 \# [3]_3) \# [1^2]_2$,

Γ_3: $([3]_1 \# [2,1]_3) \# [2]_2$,

Γ_4: $([3]_1 \# [2,1]_3) \# [1^2]_2$,

Γ_5: $([3]_1 \# [1^3]_3 \# [2]_2$,

Γ_6: $([3]_1 \# [1^3]_3 \# [1^2]_2$,

Γ_7: $([2,1]_1 \# [3]_3) \# [2]_2$,

Γ_8: $([2,1]_1 \# [3]_3) \# [1^2]_2$,

Γ_9: $([2,1]_1 \# [2,1]_3) \# [2]_2$,

Γ_{10}: $([2,1]_1 \# [2,1]_3) \# [1^2]_2$,

Γ_{11}: $([2,1]_1 \# [1^3]_3) \# [2]_2$,

Γ_{12}: $([2,1]_1 \# [1^3]_3) \# [1^2]_2$,

Γ_{13}: $([1^3]_1 \# [3]_3) \# [2]_2$,

Γ_{14}: $([1^3]_1 \# [3]_3) \# [1^2]_2$,

Γ_{15}: $([1^3]_1 \# [2,1]_3) \# [2]_2$,

Γ_{16}: $([1^3]_1 \# [2,1]_3) \# [1^2]_2$,

Γ_{17}: $([1^3]_1 \# [1^3]_3) \# [2]_2$,

Γ_{18}: $([1^3]_1 \# [1^3]_3) \# [1^2]_2$.

The group $G = \{(1)(2)(3),\ (13)(2)\}$ acts on F, the set $\{\Gamma_1, \Gamma_2, \ldots, \Gamma_{18}\}$, and partitions the elements of F into equivalence classes. The cycle index of G can be seen to be

$$P_G = \tfrac{1}{2}(S_{11}^2 S_{21} + S_{12} S_{21}) \ . \tag{6}$$

Since the number of irreducible representations of $H_1 = S_3$ is three and the number of irreducible representations of $H_2 = S_2$ is two, replacing every S_{1k} by 3 and every S_{2k} by 2, we obtain the number of classes of irreducible representations of the basis group. The number of classes is

$$\tfrac{1}{2}[3^2 \cdot 2 + 2 \cdot 3] = 12 \ .$$

The generating function for the classes is found as follows: Let α_{11}, α_{12}, and α_{13} be the weights of $[1^3]$, $[2,1]$, and $[3]$, respectively. Let α_{21} and α_{22} be the weights of $[2]$ and $[1^2]$, respectively. Then the generating function is

$$\tfrac{1}{2}[(\alpha_{11}+\alpha_{12}+\alpha_{13})^2(\alpha_{21}+\alpha_{22}) + (\alpha_{21}+\alpha_{22})(\alpha_{11}^2+\alpha_{12}^2+\alpha_{13}^2)] \ . \tag{7}$$

This on simplification yields

$$\begin{aligned}&\alpha_{11}^2\alpha_{21} + \alpha_{11}^2\alpha_{22} + \alpha_{12}^2\alpha_{21} + \alpha_{12}^2\alpha_{22} + \alpha_{13}^2\alpha_{21} + \alpha_{13}^2\alpha_{22}\\ &\quad + \alpha_{11}\alpha_{12}\alpha_{21} + \alpha_{11}\alpha_{12}\alpha_{22} + \alpha_{12}\alpha_{13}\alpha_{21} + \alpha_{12}\alpha_{13}\alpha_{22}\\ &\quad + \alpha_{11}\alpha_{13}\alpha_{21} + \alpha_{11}\alpha_{13}\alpha_{22} \ .\end{aligned} \tag{8}$$

Therefore, the classes of irreducible representations are

Γ_1': $([1^3] \# [1^3]) \# [2]$,

Γ_2': $([1^3] \# [1^3]) \# [1^2]$,

Γ_3': $([2,1] \# [2,1]) \# [2]$,

Γ_4': $([2,1] \# [2,1] \# [1^2]$,

Γ_5': $([3] \# [3]) \# [2]$,

Γ_6': $([3] \# [3]) \# [1^2]$,

Γ_7': $([1^3] \# [2,1] \# [2]$,

Γ_8': $([1^3] \# [2,1]) \# [1^2]$,

Γ_9': $([2,1] \# [3]) \# [2]$,

Γ_{10}': $([2,1] \# [3]) \# [1^2]$,

Γ_{11}': $([1^3] \# [3]) \# [2]$,

Γ_{12}': $([1^3] \# [3]) \# [1^2]$.

The corresponding inertia groups are $S_2[S_3, S_2]$, $S_2[S_3, S_2]$, $S_2[S_3, S_2]$, $S_2[S_3, S_2]$, $S_2[S_3, S_2]$, $S_2[S_3, S_2]$, $S_3^2 \times S_2$, $S_3^2 \times S_2$, $S_3^2 \times S_2$, $S_3^2 \times S_2$, $S_3^2 \times S_2$, and $S_3^2 \times S_2$, respectively. The corresponding inertia factors are S_2', S_2', S_2', S_2', S_2', S_2', S_1', S_1', S_1', S_1', S_1', and S_1'. Thus, the 18 irreducible representations of $S_2[S_3, S_2]$ are as follows:

Γ_1'': $\overparen{([1^3] \# [1^3]) \# [2]} \otimes [2]' : A_4$,

Γ_2'': $\overparen{([1^3] \# [1^3]) \# [2]} \otimes [1^2]' : A_3$,

Γ_3'': $\overparen{([1^3] \# [1^3]) \# [1^2]} \otimes [2]' : A_4'$,

Γ_4'': $\overparen{([1^3] \# [1^3]) \# [1^2]} \otimes [1^2]' : A_3'$,

Γ_5'': $\overparen{([2,1] \# [2,1]) \# [2]} \otimes [2]' : G_1$,

Γ_6'': $\overparen{([2,1] \# [2,1]) \# [2]} \otimes [1^2]' : G_2$,

Γ_7'': $\overparen{([2,1] \# [2,1] \# [1^2]} \otimes [2]' : G_1'$,

Γ_8'': $\overparen{([2,1] \# [2,1]) \# [1^2]} \otimes [1^2]' : G_2'$,

Γ_9'': $\overparen{([3] \# [3] \# [2]} \otimes [2]' : A_1$,

Γ_{10}'': $\overparen{([3] \# [3]) \# [2]} \otimes [1^2]' : A_2$,

Γ_{11}'': $\overparen{([3] \# [3]) \# [1^2]} \otimes [2]' : A_1'$,

Γ_{12}'': $\overparen{([3] \# [3]) \# [1^2]} \otimes [1^2]' : A_2'$,

Γ_{13}'': $\overparen{([1^3] \# [2,1]) \# [2]} \otimes [1]'$
$= ([1^3] \# [2,1]) \# [2] \uparrow S_2[S_3, S_2] : G_4$,

Γ_{14}'': $\overparen{([1^3] \# [2,1]) \# [1^2]} \otimes [1]'$
$= ([1^3] \# [2,1]) \# [1^2] \uparrow S_2[S_3, S_2] : G_4'$,

Γ_{15}'': $\overparen{([2,1] \# [3]) \# [2]} \otimes [1]'$
$= ([2,1] \# [3]) \# [2] \uparrow S_2[S_3, S_2] : G_3$,

Γ_{16}'': $\overparen{([2,1] \# [3]) \# [1^2]} \otimes [1]'$
$= (2,1] \# [3]) \# [1^2] \uparrow S_2[S_3, S_2] : G_3'$,

Γ_{17}'': $\overparen{([1^3] \# [3]) \# [2]} \otimes [1]' = ([1^3] \# [3]) \# [2] \uparrow S_2[S_3, S_2] : E$,

Γ_{18}'': $\overparen{([1^3] \# [3]) \# [1^2]} \otimes [1]'$
$= ([1^3] \# [3]) \# [1^2] \uparrow S_2[S_3, S_2] : E'$.

These are of dimension 1, 1, 1, 1, 4, 4, 4, 4, 1, 1, 1, 1, 4, 4, 4, 4, 2, and 2, respectively, satisfying the rule $8 \cdot 1^2 + 8 \cdot 4^2 + 2 \cdot 2^2 = 144$. The character table is shown in Table IV.

TABLE IV. The character table of $S_2[S_3, S_2]$, the NMR group of propane.

Conjugacy classes	E	(12)	(123)	(12) (67)	(123) (678)	(12) (678)	(16) (27) (38)	(173628)	(17) (2836)	(45)	(12) (45)	(123) (45)	(12) (67) (45)	(123) (678) (45)	(12) (678) (45)	(16) (27) (38) (45)	(173628) (45)	(17) (2836) (45)
Order	1	6	4	9	4	12	6	12	18	1	6	4	9	4	12	6	12	18
A_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
A_2	1	1	1	1	1	1	−1	−1	−1	1	1	1	1	1	1	−1	−1	−1
A_3	1	−1	1	1	1	−1	−1	−1	1	1	−1	1	1	1	−1	−1	−1	1
A_4	1	−1	1	1	1	−1	1	1	−1	1	−1	1	1	1	−1	1	1	−1
G_1	4	0	−2	0	1	0	2	−1	0	4	0	−2	0	1	0	2	−1	0
G_2	4	0	−2	0	1	0	−2	1	0	4	0	−2	0	1	0	−2	1	0
G_3	4	2	1	0	−2	−1	0	0	0	4	2	1	0	−2	−1	0	0	0
E	2	0	2	−2	2	0	0	0	0	2	0	2	−2	2	0	0	0	0
G_4	4	−2	1	0	−2	1	0	0	0	4	−2	1	0	−2	1	0	0	0
A_1'	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	−1
A_2'	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1
A_3'	1	−1	1	1	1	−1	−1	−1	1	−1	1	−1	−1	−1	1	1	1	−1
A_4'	1	−1	1	1	1	−1	1	1	−1	−1	1	−1	−1	−1	1	−1	−1	1
G_1'	4	0	−2	0	1	0	2	−1	0	−4	0	2	0	−1	0	−2	1	0
G_2'	4	0	−2	0	1	0	−2	1	0	−4	0	2	0	−1	0	2	−1	0
G_3'	4	2	1	0	−2	−1	0	0	0	−4	−2	−1	0	2	1	0	0	0
E'	2	0	2	−2	2	0	0	0	0	−2	0	−2	2	−2	0	0	0	0
G_4'	4	−2	1	0	−2	1	0	0	0	−4	2	−1	0	2	−1	0	0	0

TABLE V. The character table of the molecular group of the nonrigid triphenyl shown in Fig. 1. The asterisk on the permtuations indicates permutation followed by inversion.

Conjugacy classes	E	(1,3) (4,5)	(1,3) (4,5) (10, 14) (11,13)	(1,11) (2,12) (3,13) (4,14) (5,10) (6,8) (7,9)	(2,12) (1,13,3,11) (6,8) (7,9) (4,10,5,14)	(6,9)(7,8)	(1,3) (4,5) (6,9) (7,8)	(1,3) (4,5) (10,14) (11,13) (6,9) (7,8)	(1,11) (2,12) (5,10) (3,13) (4,14) (6,7) (8,9)	(2,12) (1,13,3,11) (6,7) (8,9) (4,10,5,14)	E^*	(1,3) (4,5)*	(1,3) (4,5) (10,14) (11,13)*	(1,11) (2,12) (3,13) (4,14) (5,10) (6,8) (7,9)*	(2,12) (1,13,3,11) (6,8) (7,9) (4,10,5,14)*	(6,9) (7,8)*	(1,3) (4,5) (6,9) (7,8)*	(1,3)(4,5)(10,14) (11,13) (6,9) (7,8)*	(1,11) (2,12) (5,10) (3,13) (4,14) (6,7) (8,9)*	(2,12) (1,13,3,11) (6,7) (8,9) (4,10,5,14)*
Order	1	2	1	2	2	1	2	1	2	2	1	2	1	2	2	1	2	1	2	2
A'_{1g}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
B'_{1g}	1	1	1	−1	−1	1	1	1	−1	−1	1	1	1	−1	−1	1	1	1	−1	−1
A'_{2g}	1	−1	1	−1	1	1	−1	1	−1	1	1	−1	1	−1	1	1	−1	1	−1	1
B'_{2g}	1	−1	1	1	−1	1	−1	1	1	−1	1	−1	1	1	−1	1	−1	1	1	−1
A''_{1g}	1	1	1	1	1	−1	−1	−1	−1	−1	1	1	1	1	1	−1	−1	−1	−1	−1
B''_{1g}	1	1	1	−1	−1	−1	−1	−1	1	1	1	1	1	−1	−1	−1	−1	−1	1	1
A''_{2g}	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
B''_{2g}	1	−1	1	1	−1	−1	1	−1	−1	1	1	−1	1	1	−1	−1	1	−1	−1	1
A'_{1u}	1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1
B'_{1u}	1	1	1	−1	−1	1	1	1	−1	−1	−1	−1	−1	1	1	−1	−1	−1	1	1
A'_{2u}	1	−1	1	−1	1	1	−1	1	−1	1	−1	1	−1	1	−1	−1	1	−1	1	−1
B'_{2u}	1	−1	1	1	−1	1	−1	1	1	−1	−1	1	−1	−1	1	−1	1	−1	−1	1
A''_{1u}	1	1	1	1	+1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1	1
B''_{1u}	1	1	1	−1	−1	−1	−1	−1	1	1	−1	−1	−1	1	1	1	1	1	−1	−1
A''_{2u}	1	−1	1	−1	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1	−1	1	−1	1
B''_{2u}	1	−1	1	1	−1	−1	1	−1	−1	1	−1	1	−1	−1	1	1	−1	1	1	−1
E'_g	2	0	−2	0	0	2	0	−2	0	0	2	0	−2	0	0	2	0	−2	0	0
E''_g	2	0	−2	0	0	−2	0	2	0	0	2	0	−2	0	0	−2	0	2	0	0
E'_u	2	0	−2	0	0	2	0	−2	0	0	−2	0	2	0	0	−2	0	2	0	0
E''_u	2	0	−2	0	0	−2	0	2	0	0	−2	0	2	0	0	2	0	−2	0	0

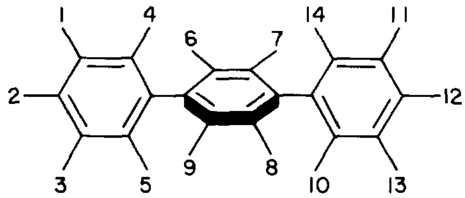

FIG. 1. The nonrigid triphenyl molecule.

IV. CERTAIN APPLICATIONS

Enough has been said about the representations of generalized wreath product groups. A number of applications of nonrigid group theory can be found in the pioneering work of Longuet-Higgins.[1] We shall illustrate one of the important applications of the generalized wreath product group in this section, namely, the derivation of the allowed electric dipole transitions for a nonrigid triphenyl shown in Fig. 1. The phenyl rings are alternately in planes perpendicular to each other. Let the rings 1 and 3 be in the set Y_1, and the ring 2 be in the set Y_2. The barrier to rotation around the C–C bond connecting two phenyl rings is very small in unsubstituted triphenyls. Therefore, even at room temperature, the triphenyl under consideration exhibits rapid internal twofold rotation. Let these internal rotations be expressed as groups C_2 acting on the protons attached to the rings in Y_1 and C_2 acting on the protons attached to the ring in Y_2. Then the rotational subgroup of the point group of the nonrigid triphenyl is $C_2[C_2, C_2]$. The full point group can be obtained by incorporating the inversion operations. The irreducible representations of the corresponding generalized wreath product can be obtained using the method outlined in Sec. III. The character table and the symmetry species are shown in Table V. Classes bearing asterisks indicate permutations followed by inversion. Since the electric dipole moment is an odd operator with respect to inversion, the allowed electric dipole transitions are

$$A'_{1g} \leftrightarrow A'_{1u},\ B'_{1g} \leftrightarrow B'_{1u},\ A'_{2g} \leftrightarrow A'_{2u},\ B'_{2g} \leftrightarrow B'_{2u},\ A''_{1g} \leftrightarrow A''_{1u},$$
$$B''_{1g} \leftrightarrow B''_{1u},\ A''_{2g} \leftrightarrow A''_{2u},\ B''_{2g} \leftrightarrow B''_{2u},\ E'_g \leftrightarrow E'_u, \text{ and } E''_g \leftrightarrow E''_u .$$

Applications of nonrigid group theory to the construction of correlation diagrams and rovibronic symmetry correlations can be found in Refs. 25 and 26, respectively.

In this paper, I tried to give a rigorous formal theory to many previous works on the symmetry groups of nonrigid molecules. We also obtained the character tables of several groups of nonrigid molecules that have not been obtained before. We extended the concept of nonrigid molecular group theory to encompass molecules having more than one "type" of "internal permutation group" using the generalized wreath product groups. Applications of the generalized wreath product group to NMR spectroscopy can be found in Refs. 5, 13, and 16(d).

ACKNOWLEDGMENTS

The author is indebted to Professor Joseph A. Shalika for many illuminating discussions. The author thanks Professor Harris J. Silverstone for his encouragement and Dr. David R. Yarkony for his encouragement and invaluable comments on the manuscript. The author is indebted to the referee for his suggestion concerning the composition law defined in the multiplication of elements of the wreath product and to include a proof for the associativity of the multiplication of the elements of wreath product groups.

APPENDIX

A generating function for the number of conjugacy classes of $S_n[H]$ is determined here. Let the number of conjugacy classes of H be s. Let a typical $(n_1, n_2, \ldots, n_s)$-tuple with $\sum_i n_i = n$ have λ_0 0's, λ_1 1's, $\ldots, \lambda_n$ n's. Then it can be shown that the number of such ordered tuples is the multinomial number

$$\binom{s}{\lambda_0 \lambda_1 \cdots \lambda_{n-1} \lambda_n},$$

such that $\lambda_0 + \lambda_1 + \cdots + \lambda_n = s$ and $1 \cdot \lambda_1 + 2\lambda_2 + \cdots + n\lambda_n = n$. Each such s-tuple will contribute the same factor $[P(0)]^{\lambda_0}[P(1)]^{\lambda_1} \cdots [P(n)]^{\lambda_n}$ to the sum $\sum_{(n)} P(n_1)P(n_2) \times P(n_2) \cdots P(n_s)$. Thus, the number of conjugacy classes of $S_n[H]$ is

$$\sum_{\substack{\lambda_0+\lambda_1+\cdots+\lambda_n=s \\ 1\lambda_1+\cdots+n\lambda_n=n}} \binom{s}{\lambda_0 \lambda_1 \cdots \lambda_{n-1} \lambda_n} [P(0)]^{\lambda_0}[P(1)]^{\lambda_1} \cdots [P(n)]^{\lambda_n} .$$

A generating function for $P(n)$ can be easily obtained (see, for example, Berge[21]). It is $F(x) = (1-x)^{-1} \times (1-x^2)^{-1}(1-x^3)^{-1} \cdots$. The coefficient of x^n in $F(x)$ gives $P(n)$.

[1] H. C. Longuet-Higgins, Mol. Phys. **6**, 445 (1963).
[2] T. Kasuya, Sci. Pap. Inst. Phys. Chem. Res. (Jpn.) **56**, 1 (1962).
[3] C. M. Woodman, Mol. Phys. **11**, 109 (1966).
[4] C. M. Woodman, Mol. Phys. **19**, 753 (1970).
[5] K. Balasubramanian, J. Chem. Phys. (to be submitted).
[6] J. Serre, Int. J. Quantum Chem. Symp. **1**, 713 (1967).
[7] J. Serre, Int. J. Quantum Chem. Symp. **2**, 207 (1968).
[8] J. Serre, Adv. Quantum Chem. **8**, 1 (1974).
[9] A. Kerber, *Lecture Notes in Mathematics* (Springer, New York, 1971), No. 240.
[10] (a) A. Kerber, *Lecture Notes in Mathematics* (Springer, New York, 1975), No. 495. (b) A. Kerber and J. Tappe, Discrete Math. **15**, 151 (1976); (c) P. Hoffman, Discrete Math. **23**, 37 (1978); (d) A. Kerber, Discrete Math. **13**, 13 (1975).
[11] A. J. Stone, J. Chem. Phys. **41**, 1568 (1964).
[12] (a) S. L. Altmann, Mol. Phys. **21**, 587 (1971); (b) S. L. Altmann, Proc. R. Soc. (London) Ser. A **298**, 184 (1967); (c) J. M. F. Gilles and J. Philippot, Int. J. Quantum. Chem. **6**, 225 (1972); **14**, 299 (1978); (d) A. Bauder, R. Meyer, and Hs. H. Gunthard, Mol. Phys. **28**, 1305 (1974); **32**, 443 (1976); (e) J. K. G. Watson, Mol. Phys. **21**, 577 (1971); (f) B. J. Dalton, *ibid*. **11**, 265 (1966); (g) H. Frei, P. Groner, A. Bauder, and Hs. H. Gunthard, *ibid*. **36**, 1469 (1978).
[13] K. Balasubramanian, Theor. Chim. Acta 51, 37 (1979).
[14] Y. Ellinger and J. Serre, Int. J. Quantum Chem. Symp. **7**, 217 (1973).
[15] C. Trindle and T. D. Bouman, Int. J. Quantum Chem. Symp. 7, 329 (1973).
[16] (a) K. Balasubramanian, Master's Thesis, Birla Institute of Technology and Science, Pilani, India (1977); (b) R. A. Davidson, Ph.D. Thesis, Pennsylvania State University (1977); (c) K. Balasubramanian, Proceedings of the 2nd International

Conference on Combinatorial Mathematics, Ann. N. Y. Acad. Sci. **319**, 33 (1978); (d) K. Balasubramanian, Theor. Chim. Acta (in press); (e) J. G. Nourse, J. Am. Chem. Soc. 101, 1210 (1979).

[17]D. Meinköhn, J. Chem. Phys. **68**, 3528, 3537 (1978); and the references given therein.

[18]A special case of this formula was used by Klein and Cowley [D. J. Klein and A. H. Cowley, J. Am. Chem. Soc. **100**, 2593 (1978)] in their general discussion on permutational isomerism with didentate ligands and other constraints using the double coset method of E. Ruch and co-workers.

[19]C. W. Curtis and I. Reiner, *Representation Theory of Finite Groups and Associative Algebras* (Interscience, New York, 1962).

[20]A. J. Coleman, in *Group Theory and its Applications*, edited by E. M. Loebl (Academic, New York, 1968), pp. 57–116.

[21]C. Berge, *Principles of Combinatonics* (Academic, New York, London, 1971).

[22]M. Hammermash, *Group Theory and Its Applications to Physical Problems* (Addison-Wesley, Reading Mass., 1962).

[23]The character table of $S_3[S_3]$ can also be found in D. E. Littlewood, *The Theory of Group Characters and Matrix Representations of Groups* (Clarendon, Oxford, 1940), p. 280. The character tables of $D_{3h}[C_3]$, $S_2[S_4]$, $S_2[S_3]$, and $S_4[S_2]$ can also be obtained in pages 282, 277, 275, and 278 of this book, respectively. The character table of $D_{3h}[C_3]$, the nonrigid molecular group of $B(CH_3)_3$, was also presented by Longuet-Higgins without a method (Cf. Ref. 1, p. 454).

[24]G. Polya, Acta Math. **68**, 145 (1937).

[25]F. Amar, M. E. Kellman, and R. S. Berry, J. Chem. Phys. **70**, 1973 (1979).

[26]A. Metropoulas and Y. N. Chiu, Chem. Phys. **36**, 113 (1979); J. Chem. Phys. **68**, 1336, 5607 (1978).