LBL-12724

CONF-810655--1

Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

Materials & Molecular Research Division

To be presented at the SIAM Conference on Applications of Discrete Mathematics, Troy, NY, June 10-12, 1981

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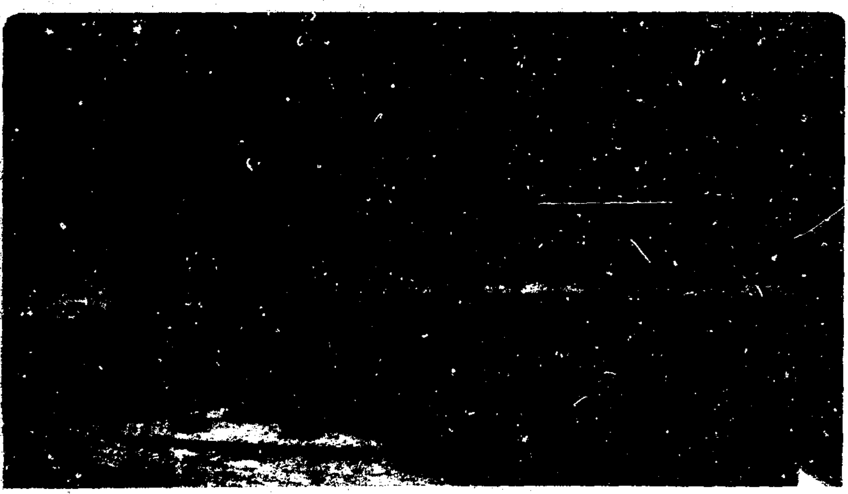
MASTER

May 1981



Prepared for the U.S. Department of Energy under Contract W-7405-ENG-48

Symmetry Operators of Generalized Wreath Products and Their Applications to Chemical Physics

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Symmetry operators of generalized wreath product groups are formulated. Several applications of these operators to non-rigid molecular problems in chemical physics are outlined.

* Part of the work presented here was done at The Johns Hopkins University, Baltimore, MD 21218

This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under Contract No. W-7405-ENG-48.

I. Introduction

In recent years generalized wreath product groups were used as efficient representations of symmetries of molecules exhibiting large amplitude non-rigid motions,[1,2] NMR spin hamiltonians,[3] etc. By the term 'large amplitude' we mean amplitudes large in the ordinary experimental NMR scale. Randić,[4-7] Balaban[8,9] and the present author[10] studied the symmetry groups of graphs of chemical interest. The symmetry groups of a number of chemically interesting graphs can be embedded into wreath or generalized wreath products. Balaban and coworkers[11,12] and Randić[7] have recognized the use of wreath products in such chemical applications.

The generalized wreath product groups have special structures that provide for elegant derivation of physically interesting quantities. The generalized character cycle indices (GCCI's) of these groups can be obtained in terms of the composing groups. These GCCI's are the generators of spin species, NMR spin multiplets and nuclear spin statistical weights. The nuclear spin statistical weights of the rovibronic levels are of fundamental importance in molecular spectroscopy. They provide information on the intensities of allowed inter-rovibronic transitions. Thus the combinational numbers generated from the GCCI's are prints of the intensity ratios of the various peaks appearing in a molecular spectra.

In this paper we will first briefly outline the preliminary combinatorial concepts. In Sec. III formalisms related to the symmetry operators of generalized wreath products are outlined. In Sec. IV applications to the symmetry groups of non-rigid molecules is considered. Sec. V concludes with generalized isomer enumerations. For several chemical applications of graph theory the readers are referred to the book by Balaban[13] and related papers by Randić,[14-20] Balaban,[21-25] the present author,[26-34] and Dolhaine.[35]

II. Preliminaries

Let D and R be finite sets and let $|D|$ and $|R|$ denote the number of elements in D and R, respectively. Let G be a permutation group acting on D. Consider the set of maps from D to R. Let R^D denote the set of all such maps. In several situations we may need to consider maps from the cartesian product A x B (A and B being two finite sets) to R or from the union of several such cartesian products to R. The permutation group G acting on D induces permutations on $F = R^D$ by the following recipe.

$$gf(i) = f(g^{-1}i) \qquad \text{for} \qquad i\epsilon D: \; f\epsilon R^D.$$

Let V be a vector space over a field K of characteristic zero with dim $V = |R| = r$ and let $e_1, e_2, \ldots e_r$ be a standard basis of V. With each $f\epsilon R^D$ we can associate the tensor product $e_f = e_{f(1)} \otimes e_{f(2)} \otimes \ldots \otimes e_{f(d)}$ and the set of such tensors forms the basis of the d^{th} tensor product of V. For a $g\epsilon G$ we define the permutation operator $P(g)$ with respect to this basis set by $P(g)e_f = e_{gf} = e_{gf(1)} \otimes e_{gf(2)} \otimes \ldots \otimes e_{gf(d)} = e_{f(g^{-1}1)} \otimes e_{f(g^{-1}2)} \otimes \ldots \otimes e_{f(g^{-1}d)}$. Let $\omega: G \to F$ be a non-zero homomorphism (i.e., $\omega(g_1g_2) = \omega(g_1)\omega(g_2)$, a character of degree 1). We define a symmetry operator T_G as

$$T_G = \frac{1}{|G|} \sum_{g\epsilon G} \omega(g)P(g).$$

Consider a map W from F to K, $W: F \to K$ which is also a constant on the orbits resulting from the action of G on F. If W also satisfies the following property for every f, it is referred to as a weight function.

$$W(f) = \prod_{i=1}^{d} w(f(i))$$

where w is a function, $w: R \to K$. W(f) is also referred to as a weight of a function in combinatorics book.[38]

Consider the subspace V_x^d of V^d, (where V^d is the d^{th} tensor product of V) spanned by all tensors $S_x = \{e_f : W(f) = x \in K\}$. Let the restrictions of the operators T_G and $P(g)$ to the space V_x^d be $T_G^{\,x}$ and $P_x(g)$, respectively. Now, define the weighted permutation operator $P_W(g)$ and the weighted symmetry operator T_G^W with the weight W as

$$P_W(g) = \bigoplus_{x \in K} x\, P_x(g)$$

$$T_G^W = \bigoplus_{x \in K} x\, T_G^x$$

where $\oplus$ denotes a direct sum. (See Ref. 41 for a definition of direct sum.) If one considers a matrix representation of $P_W(g)$ then we have

$$\mathrm{tr}\, P_W(g) = \sum_f^{(g)} W(f)$$

where the sum is taken over all f for which $gf = f$. Williamson[36] proved the following theorem.

<u>Theorem 1</u>:

$$T_G^W = \frac{1}{|G|} \sum_{g \in G} \omega(g)\, P_W(g).$$

Thus

$$\mathrm{tr}\, T_G^W = \frac{1}{|G|} \sum_{g \in G} \omega(g)\, \mathrm{tr}(P_W(g))$$

$$= \frac{1}{|G|} \sum_{g \in G} \omega(g) \sum_f^{(g)} W(f).$$

If one defines the generalized character cycle index (GCCI) of a group G with character χ as corresponding to the irreducible representation Γ, as

$$P_G^{\chi}(s_1,s_2,\ldots) = \frac{1}{|G|}\sum_{g\in G}\chi(g)\, s_1^{b_1} s_2^{b_2}\ldots$$

where $s_1^{b_1} s_2^{b_2}\ldots$ is a representation of a typical permutation $g\in G$ having b_1 cycles of length 1, b_2 cycles of length 2, etc. Then by theorem 1 and the preliminary combinatorial results in reference 38,

$$\mathrm{tr}\ T_G^W = P_G^{\chi}\Big(\sum_{r\in R} w(r),\ \sum_{r\in R}(w(r))^2,\ldots\Big).$$

We now proceed to the symmetry operators of generalized wreath products.

III. Symmetry Operators of Generalized Wreath Product Groups

Let a set $\Omega = \{1,2,\ldots,n\}$ be partitioned into the mutually disjoint sets $Y_1, Y_2,\ldots,Y_t$. Let G be a permutation group acting on Ω such that all its orbits are within the same Y-sets. Let $H_1, H_2,\ldots,H_t$ be t permutation groups and let Π_i be a map from Y_i to H_i (for $i = 1,2,\ldots,t$). Then the set $\{(g;\Pi_1,\Pi_2,\ldots\Pi_t)|g\in G,\ \Pi_i:Y_i\rightarrow H_i\}$ is called a generalized wreath product and is denoted as $G[H_1,H_2,\ldots,H_t]$. Let G_i be the set of all cycle products contained in the set Y_i. It is shown in ref. 1 that G_i forms a group. The multiplication of the elements of generalized wreath product is defined as follows:

$$(g;\Pi_1,\Pi_2,\ldots,{}_t)\cdot(g';\Pi_1',\Pi_2',\ldots,\Pi_t') = (gg';\Pi_1\Pi_{1_{g_1}}'\ \Pi_2\Pi_{2_{g_2}}',\ldots\ldots,\Pi_t\Pi_{t_{g_t}}')$$

with

$$\Pi_{i_{g_i}}'(j) = \Pi_i'(g_i^{-1}j)$$

where g_i is the cycle product of g contained in Y_i. The product $(H_1^{m_1*} \times H_2^{m_2*} \times \ldots \times H_t^{m_t*}).G'$ is a permutation representation of $G[H_1,H_2,\ldots H_t]$ where $H_i^{m_i*} = H_{i1} \times H_{i2} \times \ldots \times H_{im_i}$,

$G' = \{(g;e_1,e_2,\ldots e_t) | g \in G,\ e_i(j) = 1_{H_i}$ (the identity of Group H_i)$\forall j \in Y_i\}$

H_{ij} is a copy of the group H_i. The special case of this group with $t=1$ is the well-known wreath product denoted as $G[H]$.

Let the irreducible representations of $H_1^{m_1*} \times H_2^{m_2*} \times \ldots \times H_t^{m_t*}$ be denoted as $F_1^{m_1*} \# F_2^{m_2*} \# \ldots \# F_t^{m_t*}$ where $F_i^{m_i*}$ is the outer tensor product $F_{i1} \# F_{i2} \# \ldots \# F_{im_i}$, with F_{ij} being an irreducible representation of H_i. The group G acts on the set of $\#_i F_i^{m_i*}$'s and partitions them into equivalence classes. The inertia group of each such class should be determined where the inertia group consists of the set of those permutations satisfying the following property.

$$G_\Gamma[H_1,H_2,\ldots H_t] = \{(g;\Pi_1,\Pi_2,\ldots \Pi_t) / \Gamma^{(g;\Pi_1,\Pi_2,\ldots,\Pi_t)} \sim \Gamma\}$$

where $$\Gamma = \#_i F_i^{m_i*}$$

with

$$F^{*(g;\Pi_1,\Pi_2,\ldots \Pi_t)}(e;\Pi_1',\Pi_2',\ldots,\Pi_t') = F^*(g;\Pi_1\ \Pi_2\ \ldots \Pi_t)^{-1}(e;\Pi_1'\ \Pi_2',\ldots,\Pi_t')$$
$$(g;\Pi_1,\Pi_2,\ldots \Pi_t).$$

A permutation representation of the inertia Group $G_\Gamma[H_1,H_2,\ldots,H_t]$ is $(H_1^{m_1*} \times H_2^{m_2*} \times \ldots \times H_t^{m_t*}).G_\Gamma'$ where G_Γ' is known as the inertia factor. If one knows the representation matrices of $(F_1^{m_1*} \# F_2^{m_2*} \# \ldots \# F_t^{m_t*})$ $(e;e_1,e_2,\ldots,e_t)$ it is possible to find the representation matrices of $\widetilde{F_1^{m_1*} \# F_2^{m_2*} \# \ldots \# F_t^{m_t*}}(g;e_1,e_2,\ldots,e_t)$ by a suitable permutation of the columns of $\#_1 F_1^{m_{1*}}$ determined by g^{-1} as described in reference 1. The group G acting on Ω must be intransitive. This is implicit in partitioning the set Ω into disjoint sets $Y_1, Y_2, \ldots, Y_t$ and stipulating that every $g \varepsilon G$ has all its orbits within the same Y-sets. Let $T_1, T_2, \ldots, T_t$ be t sets. T's are usually referred to as types. Then the generalized wreath product $G[H_1, H_2, \ldots, H_t]$ with H_i acting on T_i acts on $\bigcup_{i=1}^{t} Y_i \times T_i$. A typical $(g; \Pi_1, \Pi_2, \ldots, \Pi_t)$ $\varepsilon G[H_1, H_2, \ldots, H_t]$ acts on $\bigcup_i Y_i \times T_i$ as follows:

$$(g; \Pi_1, \Pi_2, \ldots, \Pi_t)(y;t) = (gy : \Pi_i(y)t) \quad \text{if} \quad y \varepsilon Y_i \quad \text{and} \quad t \varepsilon T_i .$$

Consider the set of maps from $\bigcup_{i=1}^{t} Y_i \times T_i$ to a set R and let such a set of maps be denoted as

$$R^{\bigcup_i Y_i x T_i} .$$

The action of $G[H_1, H_2, \ldots, H_t]$ on $\bigcup_i Y_i x T_i$ in turn induces permutations on $R^{\bigcup_i Y_i x T_i}$, for a $(g; \Pi_1, \Pi_2, \ldots, \Pi_t)$ $\varepsilon G[H_1, H_2, \ldots, H_t]$ and $f \varepsilon R^{\bigcup_i Y_i x T_i}$

$$(g; \Pi_1, \Pi_2, \ldots, \Pi_t) f(y,t) = \Pi_i(g^{-1}y) f(g^{-1}y, t) \quad \text{if} \quad y \varepsilon Y_i \quad \text{and} \quad t \varepsilon T_i .$$

Let $W : R^{\bigcup_i Y_i x T_i} \to K$ be defined by

$$W(f) = \prod_{\substack{(y,t) \varepsilon Y_i x T_i \\ i=1,t}} w(f(y,t))$$

where $w : R \to K$. W is a weight function which is also a constant on the orbits of $G[H_1, H_2, \ldots, H_t]$.

Let $\lambda_i : H_i \to K$, $\chi : G \to K$ be characters of degree 1. For a $\Pi_i \varepsilon H_i^{Y_i}$ define $\bar{\lambda}_i(\Pi_i) = \prod_{y \varepsilon Y_i} \lambda_i(\Pi_i(y))$. This is just a $|Y_i|$-fold repeated product of λ_i. Let $\omega(g; \Pi_1, \Pi_2, \ldots, \Pi_t)$ be defined by $\omega(g; \Pi_1, \Pi_2, \ldots, \Pi_t) = \chi(g) \bar{\lambda}_1(\Pi_1) \bar{\lambda}_2(\Pi_2) \ldots \bar{\lambda}_t(\Pi_t)$. Then note that $\omega(g; \Pi_1, \Pi_2, \ldots, \Pi_t)$ is a character of $G[H_1,H_2,\ldots,H_t]$ with degree 1.

Let V be a vector space over the field K with dim $V = |R|$. Define symmetry operator T_{H_i}, whose range space is $\otimes^{|Y_i|} V$, as

$$T_{H_i} = \frac{1}{|H_i|} \sum_{h \in H_i} \lambda_i(h) P(h).$$

Let the vector space spanned by the basis $\{e_{f_i} : f_i \in \bar{\Delta}_H^{\lambda_i}\}$ be denoted as $V_{H_i}^{\lambda_i}$. $\bar{\Delta}_{H_i}^{\lambda_i} = \{\gamma \in R^D | \sum_{\sigma \in H_i(\gamma)} \lambda_i(\sigma) \neq 0\} \cdot H_i(\gamma) = \{h | h\gamma = \gamma,\ h \in H_i\}$. Then the symmetry operator of G can be defined over the tensor product space

$$\otimes^{|Y_1|} V_{H_1}^{\lambda_1} \otimes^{|Y_2|} V_{H_2}^{\lambda_2} \otimes \ldots \otimes^{|Y_t|} V_{H_t}^{\lambda_t} \text{ by } T_G = \frac{1}{|G|} \sum_{g \in G} \chi(g) P(g).$$

With ω defined as above the symmetry operator $T_{G[H_1,H_2,\ldots,H_t]}$ can be defined as

$$T_{G[H_1,H_2,\ldots,H_t]} = \frac{1}{|G[H_1,H_2,\ldots,H_t]|} \sum \omega(g;\Pi_1,\Pi_2,\ldots,\Pi_t) P(g:\Pi_1,\Pi_2,\ldots,\Pi_t)$$

In this set up one can generalize Williamson's theorem[38] to theorem 2 stated below for abelian characters.

Theorem 2: The weighted symmetry operators $T^{\omega}_{G[H_1,H_2,\ldots,H_t]}$, T^{ω}_G, $T_{H_1^{Y_1}}$, $T_{H_2^{Y_2}}$, $\ldots T_{H_t^{Y_t}}$ are related as follows.

$$T^{\omega}_{G[H_1,H_2,\ldots,H_t]} = T^{\omega}_G \, T_{H_1^{Y_1}} \, T_{H_2^{Y_2}} \cdots T_{H_t^{Y_t}}.$$

where $T_{H_i^{Y_i}}$ is the symmetry operator which corresponds to the group $H_i^{Y_i}$.

If now one follows Williamson's method[38] of taking traces it can be shown that

$$\mathrm{tr}\ T^{\Omega}_{G[H_1,H_2,\ldots H_t]} = P^{\omega}_{G[H_1,H_2,\ldots H_t]}(s_k \to \sum_{r\in R} w^k(r))$$

where $P^{\omega}_{G[H_1,H_2,\ldots,H_t]}$ is obtained as follows.

Let $\omega(g;\Pi_1,\Pi_2,\ldots,\Pi_t) = \chi(g)\bar{\lambda}_1(\Pi_1)\bar{\lambda}_2(\Pi_2)\ldots\bar{\lambda}_t(\Pi_t)$. Define $P^{\chi}_G = \frac{1}{|G|}\sum_{g\in G}\prod_i\prod_j \chi(g)s_{ij}^{C_{ij}(g)}$ where $C_{ij}(g)$ is the number of j-cycles of g in the set Y_i. Let $Z^{\lambda_i}_{ij} = Z^{\lambda_i}_i(s_k \to s_{kj})$ where the subscript on the s-variables are products. Then

$$P^{\omega}_{G[H_1,H_2,\ldots,H_t]} = P^{\chi}_G(s_{ij} \to Z^{\lambda_i}_{ij}).$$

Let us illustrate Theorem 2 with a simple example from NMR groups, namely, the NMR group of propane, $S_2[S_3,S_2]$.

Consider the irreducible representation $([3]\#[3])\#[2] \otimes [1^2]'$ of $S_2[S_3,S_2]$. This is an one-dimensional representation.

$$P^{[1^2]}_G = \frac{1}{2}(s_{11}^2\ s_{21} - s_{21}s_{12})$$

$$Z_{11} = \frac{1}{6}(s_1^3 + 2s_3 + 3s_1s_2)$$

$$Z_{12} = \frac{1}{6}(s_2^3 + 2s_6 + 3s_2s_4)$$

$$Z_{21} = \frac{1}{2}(s_1^2 + s_2)$$

$$P^{\omega}_{G[H_1,H_2,\ldots,H_t]} = P^{[1^2]}_{G}(s_{ij} \to Z_{ij})$$

$$= \tfrac{1}{2}[\tfrac{1}{36}\{s_1^3 + 2s_3 + 3s_1s_2\}^2 \cdot \tfrac{1}{2}(s_1^2 + s_2)$$

$$- \tfrac{1}{6}(s_2^3 + 2s_6 + 3s_2s_4) \cdot \tfrac{1}{2}(s_1^2 + s_2)]$$

$$= \tfrac{1}{144}[s_1^8 + 4s_1^2s_3^2 + 15s_1^4s_2^2 + 4s_1^5s_3 + 16s_1^3s_2s_3 + 7s_1^6s_2$$

$$+ 4s_2s_3^2 + 3s_1^2s_2^3 + 12s_1s_2^2s_3 - 12s_1^2s_6 - 18s_1^2s_2s_4$$

$$- 6s_2^4 - 12s_2s_6 - 18s_2^2s_4].$$

Thus $\operatorname{tr} T^{\omega,\Gamma}_{G[H_1,H_2,\ldots,H_t]}$ with Γ: $([3]\#[3])\#[2] \otimes [1^2]'$

$$= \tfrac{1}{144}[(\sum_{r\in R} w(r))^8 + 4(\sum_{r\in R} w(r))^2(\sum_{r\in R} w^3(r))^2 + 15(\sum_{r\in R} w(r))^4$$

$$\times (\sum_{r\in R} w^2(r))^2 + 4(\sum_{r\in R} w(r))^5(\sum_{r\in R} w^3(r)) + 12(\sum_{r\in R} w(r))^3$$

$$\times (\sum_{r\in R} w^2(r))(\sum_{r\in R} w^3(r)) + 7(\sum_{r\in R} w(r))^6(\sum_{r\in R} w^2(r))$$

$$+ 4(\sum_{r\in R} w^2(r))(\sum_{r\in R} w^3(r))^2 + 3(\sum_{r\in R} w(r))^2(\sum_{r\in R} w^2(r))^3$$

$$+ 12(\sum_{r\in R} w(r))(\sum_{r\in R} w^2(r))^2(\sum_{r\in R} w^3(r)) - 12(\sum_{r\in R} w(r))^2(\sum_{r\in R} w^6(r))$$

$$- 18(\sum_{r\in R} w(r))^2(\sum_{r\in R} w^2(r))(\sum_{r\in R} w^4(r)) - 6(\sum_{r\in R} w^2(r))^4$$

$$- 12(\sum_{r\in R} w^2(r))(\sum_{r\in R} w^6(r)) - 18(\sum_{r\in R} w^2(r))^2(\sum_{r\in R} w^4(r))].$$

Let the inertia group of a representation $F^* = F_1^{m_1*} \# F_2^{m_2*} \# \ldots \# F_t^{m_t*}$ be $G_{F*}[H_1,H_2,\ldots,H_t]$ and let $G^*_{F'}$ be the corresponding inertia factor. Then we have the following generalization for non-abelian characters.

Define $P_{G_F^*}$ to be

$$P^{\chi}_{G_F^*} = \frac{1}{|G_F^*|} \sum_{g\in G_F^*} \prod_i \prod_j \chi(g)\, s_{ij}^{C_{ij}(g)}$$

where $C_{ij}(g)$ denotes the number of j-cycles of g in the set Y_i, where Y_i is defined as in Sec. III, and χ is the character of the representation F of the group G'_{F*} equivalent to F' of G'_{F*} appearing in the representation

$$\Gamma = (F_1^{m_1*} \# F_2^{m_2*} \# \cdots \# F_t^{m_t*}) \otimes F' \uparrow G[H_1,H_2,\ldots,H_t].$$

Let $Z_{ij}^{\lambda_k}$ be defined as discussed above, but now λ_k is defined by the representations appearing in the outer tensor product $F_i^{m_i*}$. Then

$$P^{\Gamma}(G[H_1,H_2,\ldots,H_t]) = P^{\chi}_{G_{F*}}(s_{ij} \rightarrow Z_{ij}^{\lambda_k})$$

if this j-cycle in Y_i is constituted by j-copies of the representation whose character is λ_k. The corresponding generating function is obtained by the following substitution:

$$G\cdot F\cdot = P^{\Gamma}(G[H_1,H_2,\ldots,H_t])(s_k \rightarrow \sum_{r\in R} w^k(r))$$

Let us illustrate the above procedure with two examples of nonabelian characters from the group $S_2[S_3,S_2]$.

Let Γ be $([2,1] \# [2,1]) \# [1^2] \otimes [1^2]' \uparrow S_2[S_3,S_2]$. The inertia group of $[2,1] \# [2,1] \# [1^2]$ is $S_2[S_3,S_2]$. The cycle index of the group S_2 isomorphic to the inertia factor with the character which corresponds to the irreducible representation $[1^2]$ is

$$P_{S_2}^{[1^2]} = \frac{1}{2}(s_{11}^2 s_{21} - s_{21}s_{12})$$

$$Z_{11}^{[2,1]} = \frac{1}{3}(s_1^3 - s_3)$$

$$Z_{12}^{[2,1]} = \frac{1}{3}(s_2^3 - s_6)$$

$$Z_{21}^{[1^2]} = \frac{1}{2}(s_1^2 - s_2).$$

Thus

$$P^{\Gamma}(S_2[S_3,S_2] = \frac{1}{2}[\frac{1}{9}(s_1^3 - s_3)^2 \cdot \frac{1}{2} \cdot (s_1^2 - s_2)$$

$$- \frac{1}{2}(s_1^2 - s_2) \cdot \frac{1}{3} \cdot (s_2^3 - s_6)]$$

$$= \frac{1}{144}[4s_1^8 - 8s_1^5 s_3 + 4s_1^2 s_3^2 - 4s_1^6 s_2 + 8s_1^3 s_2 s_3$$

$$- 4s_2 s_3^2 - 12s_1^2 s_2^3 + 12s_2^4 + 12s_1^2 s_6 - 12s_2 s_6].$$

Let Γ be $[1^3] \# [2,1] \# [2] \otimes [1]' \uparrow S_2[S_3,S_2]$. For this case the inertia group is $S_3 x S_3 x S_2$ and hence the inertia factor is the trivial group containing only the identity. In fact, Γ is equivalent to $[1^3] \# [2,1] \# [2] \uparrow S_2[S_3,S_2]$.

$$P_{S_1}^{[1]} = s_{11}^2 s_{21} \quad \text{(corresponds to (1)(3)(2))}$$

$$Z_{11}^{[1^3]} = \frac{1}{6}(s_1^3 + 2s_3 - 3s_1 s_2)$$

$$Z_{11}^{[2,1]} = \frac{1}{3}(s_1^3 - s_3)$$

$$Z_{21}^{[2]} = \frac{1}{2}(s_1^2 + s_2)$$

$$P_{S_2[S_3,S_2]}^{\Gamma} = \frac{1}{6}(s_1^3 + 2s_3 - 3s_1 s_2) \cdot \frac{1}{3} \cdot (s_1^3 - s_3) \cdot \frac{1}{2}(s_1^2 + s_2)$$

(The first factor in the product $s_{11}s_{11}$ is a consequence of the first representation in the outer product $[1^3] \# [2,1]$ while the second is a result of [2.1]. Hence the above substitution.) The corresponding generating functions can be readily obtained for both the representations.

IV. Applications to Non-Rigid Molecules

The GCCI's of generalized wreath products can thus be obtained in terms of the GCCI's of the composing groups. Consequently, characters of all the classes with the same cycle type of the generalized wreath product can be generated from character tables of groups of much lower order. This has an important application in obtaining the character tables of the symmetry groups of non-rigid molecules which are in general, generalized wreath product groups.[1] Note that the coefficient of $x_1^{b_1} x_2^{b_2}$... (x's are dummy symbols like s') in P_G^{Γ} which can be obtained in terms of $P_{G_{F*}}^{\chi}$ and $Z_{ij}^{\lambda_k}$'s gives the sum of characters of elements of $G[H_1,H_2,\ldots,H_t]$ with the same cycle type. Since all the elements in the same conjugacy class have the same cycle type the coefficient of $x_1^{b_1} x_2^{b_2}$...gives

$$\sum_C \chi(C)\ |C|$$

where the sum is taken over all C with the same cycle type $x_1^{b_1} x_2^{b_2}\ldots$. $\chi(C)$ is the character of χ in the conjugacy class C and $|C|$ is the order of the conjugacy class C. When there is only one conjugacy class with the same cycle type $x_1^{b_1} x_2^{b_2}$...(which is very often the case) the coefficient of $x_1^{b_1} x_2^{b_2}$..gives $\chi(C)\ |C|$ and thus the character $\chi(C)$ is generated. When there are more than one conjugacy classes with the same cycle type, if we determine the characters of all but one conjugacy class with the methods outlined in reference 1, using the coefficient of $x_1^{b_1} x_2^{b_2}$...in $P^{\Gamma}(G[H_1,H_2,\ldots,H_t])$ the character of the last conjugacy class can be determined. In practice for several wreath products and generalized wreath products, at most 2 or 3 conjugacy classes have the same cycle type and several conjugacy classes have the unique cycle type. Thus $P^{\Gamma}(G[H_1,H_2,\ldots,H_t])$, which is obtained very elegantly and easily provides for inventories of characters of all the irreducible representations of wreath and generalized wreath products.

We now illustrate this method with examples. We give two examples, namely, $C_2[C_3]$ and $S_2[S_4]$ where there is no 1-1 correspondence between cycle representation and conjugacy classes. In table 1, the character table of the cyclic group C_3 is shown with γ_1 and γ_2 treated as components of the degenerate representation E. Table 2 shows the various GCCI's of the group C_3. The two GCCI's of the group C_2 are readily obtained. The irreducible representations of $C_2[C_3]$ and their GCCI's are shown in table 3. They were obtained in terms of the GCCI's of C_3 shown in table 2 and those of C_2. For example, the GCCI P^{Γ_2} for $\Gamma_2 = (A_1 \# A_1) \odot [1^2]'$ is given by the following substitutions:

$$P^{[1^2]} = \frac{1}{2}\,(x_{11}^2 - x_{12}) \quad \text{(There is only one Y-set)}$$

$$Z_{11}^{A_1} = \frac{1}{3}\,(x_1^3 + 2x_3) \quad \text{(from table 2)}$$

$$Z_{12}^{A_1} = \frac{1}{3}\,(x_2^3 + 2x_6)$$

Thus

$$\begin{aligned} P_2^{\Gamma} &= P^{[1^2]}\,(x_{ij} \to Z_{ij}^{\lambda_k}) \\ &= \tfrac{1}{2}[\tfrac{1}{9}\,\{x_1^3 + 2x_3\}^2 - \tfrac{1}{3}\,(x_2^3 + 2x_6)] \\ &= \tfrac{1}{18}\,(x_1^6 + 4x_1^3x_3 + 4x_3^2 - 3x_2^3 - 6x_6). \end{aligned}$$

There are 2 conjugacy classes with the cycle type $x_1^3x_3$, 3 conjugacy classes with the cycle type x_3^2, 2 conjugacy classes with the cycle type x_6 and all other cycle types have unique conjugacy classes. Thus if the character of the conjugacy class (123) in Γ_2 is determined by the method in reference 1 to be 1, then the character of the conjugacy class (132) is determined as 1 using the GCCI since the coefficient of $x_1^3x_3$ is +4 in 18 P^{Γ_2}. The characters of E and (14)(25)(36) are immediately determined using GCCI's. The character table thus obtained is shown in table 4. The complete character table of the PI group can be obtained by including the inversion operations as a semidirect product. Another non-trivial example is the group $S_2[S_4]$. The character table of S_4 and the GCCI's of S_4 are shown in tables 5 and 6, respectively. Table 7 shows the GCCI's of the 20 irreducible representations of $S_2[S_4]$ obtained using the method developed in this paper. The group $S_2[S_4]$ has 2 conjugacy classes with the cycle type $x_1^4x_2^2$, 2 classes with the cycle type x_4^2, 2 classes with the cycle type $x_2^2x_4$ and 2 with the cycle type x_2^4. The rest of the 12 conjugacy classes have unique cycle types. Thus P^{Γ}'s of $S_2[S_4]$ generate the characters of these 12 conjugacy classes immediately, while the characters of other conjugacy classes are determined using P^{Γ} and by knowing the character of one of the conjugacy classes with the method in reference 1. The character table thus obtained is shown in table 8. The conjugacy classes, order of each conjugacy class and the representatives of each conjugacy class are obtained using the method in reference 1. Table 8 is in agreement with the compound character table, [8] + [62] + [4^2] in reference 39. $C_2[C_3]$ is the rotational subgroup of non-rigid ethane. The fact that $S_2[S_4]$ is the NMR group of bicyclobutadienyl sandwich complex can be seen using the diagrammatic technique for the characterization of the NMR group of molecules presented in ref. 3. The permutation representation of the conjugacy classes were obtained using the permutation representation of the wreath product groups outlined in sec 2 and ref. 1.

As a last example to illustrate how the GCCI's of wreath products can be obtained, consider the third GCCI in table 7. The irreducible representation under consideration is $[4]\ \#\ [31] \uparrow S_2[S_4]$. The inertia factor of $[4]\ \#\ [31]$ is S_1, the group containing just (1) (2). The cycle index corresponding to the only identity representation [2] of this group is

$$P^{[2]} = x_{11}^2.$$

From table 6 we obtain,

$$Z_{11}^{[4]} = 1/24(x_1^4 + 6x_1^2x_2 + 8x_1x_3 + 6x_4 + 3x_2^2)$$

$$Z_{11}^{[31]} = 1/24(3x_1^4 + 6x_1^2x_2 - 6x_4 - 3x_2^2)$$

Therefore, for $\Gamma_3 = [4]\ \#\ [31] \uparrow S_2[S_4]$, P^{Γ_3}, is

$$P^{\Gamma_3} = 1/24(x_1^4 + 6x_1^2x_2 + 8x_1x_3 + 6x_4 + 3x_2^2) \cdot 1/24(3x_1^4 + 6x_1^2x_2 - 6x_4 - 3x_2^2)$$

$$= 1/576(3x_1^8 + 24x_1^6x_2 + 24x_1^5x_3 + 12x_1^4x_4 + 42x_1^4x_2^2 + 48x_1^3x_2x_3$$

$$- 24x_1x_2^2x_3 - 48x_1x_3x_4 - 36x_4^2 - 36x_2^2x_4 - 9x_2^4).$$

Hence 1152 P^{Γ_3} is the expression shown in table 7. From this expression the character corresponding to all the conjugacy classes can be immediately determined except the conjugacy classes with the cycle types $x_1^4x_2^2$, x_4^2, $x_2^2x_4$, and x_2^4. For example, the character corresponding the conjugacy class (12) is 1/12 times the coefficient of $x_1^6x_2$ in 1152 P^{Γ_3}. The multiplication factor is 1/12 because the order of this conjugacy class is 12. Thus, this character is 48/12=4. The character corresponding to the conjugacy classes with the cycle types $x_1^4x_2^2$, etc., can be determined if the character of one of the conjugacy classes of the same cycle type is known.

V. Generalized Isomer Enumerations

One of the interesting chemical applications of combinatorics is the enumeration of chemical isomers which are equivalence classes of maps from the set of vertices of a chemical graph to chemical substituents. Several papers[11-35] have appeared in both mathematical and chemical literature ever since the appearance of the paper of Pólya.[40] In this section we consider an important generalization using the formalism in sec II.

The complete interconversions obtainable by the allowed symmetry operations are best described by the irreducible representations contained in each equivalence class formed by isomers. Each isomer or a pattern (in Pólya terminology) is a representative of the set of functions that are transformable into one another by the action of the molecular symmetry group. The set of functions in any equivalence class transforms as a reducible representation and it will be interesting to know the irreducible representations contained in each pattern. The GCCI's introduced in earlier sections with Pólya substitution are the generators of irreducible representations contained in patterns. The coefficient of a typical term $w_1^{b_1} w_2^{b_2}$....in the GCCI corresponding to the irreducible representation Γ generates the frequency of occurrence of Γ in the set of functions with the weight $w_1^{b_1}w_2^{b_2}$...

Let us illustrate the above method with generalized isomer enumeration of non-rigid hydrazine molecule. Replace the protons of this molecule by the substituents a and b so that the chemical formula is $N_2a_2b_2$. The rotational subgroup of the non-rigid molecule is described by the wreath product $S_2[S_2]$.[1] The GCCI's of the various irreducible representations of $S_2[S_2]$ with labels in accordance to chemical literature are in table 9.

If we replace each x_k by $\sum(w(r))^k$ we obtain generators of generalized isomer enumerations. Such generators are shown below.

$$\mathrm{G.F.}^{A_1} = P_G^{A_1}(x_k \to a^k + b^k)$$
$$= a^4 + a^3b + 2a^2b^2 + ab^3 + b^4.$$

$$\mathrm{G.F.}^{B_1} = P_G^{B_1}(x_k \to a^k + b^k)$$
$$= a^3b + a^2b^2 + ab^3$$

$$\mathrm{G.F.}^{E} = P_G^{E}(x_k \to a^k + b^k)$$
$$= a^3b + a^2b^2 + ab^3$$

$$\mathrm{G.F.}^{B_2} = P_G^{B_2}(x_k \to a^k + b^k)$$
$$= a^2b^2$$

$$\mathrm{G.F.}^{A_2} = P_G^{A_2}(x_k \to a^k + b^k) = 0.$$

The coefficient of a^2b^2 in the generator corresponding to an irreducible representation Γ gives the number of times Γ occurs in the set of functions with the weight a^2b^2. The generator corresponding to the totally symmetric representation is the generator of patterns. Thus the coefficient of a^2b^2 in the A_1-generator shows that there are 2 isomers (patterns) for this molecule. The 2 functions corresponding to the isomer I (in table 10) transform as $A_1 \oplus B_1$ as generated by GCCI's. The functions which are in the equivalence class formed by the isomer II transform as $A_1 \oplus E \oplus B_2$. Equivalently, the symmetry operations of this molecule transform the maps from 4 vertices of the hydrazine to substituents a and b with the weight a^2b^2 into 2 equivalence classes. Each class splits into direct sum of irreducible representations $A_1 \oplus B_1$ and $A_1 \oplus B_2 \oplus E$, respectively.

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Table Captions

Table 1. Character table of the cyclic group C_3. γ_1 and γ_2 are the components of the degenerate representation E.

Table 2. GCCI's of the cyclic group C_3. Note that the sum of the GCCI's of γ_1 and γ_2 is the GCCI of E.

Table 3. GCCI's of $C_2[C_3]$ obtained using the procedure outlined in this paper from the GCCI's of C_2 and C_3.

Table 4. Character table of $C_2[C_3]$ generated using the GCCI's in table 3 and the methods outlined in reference

Table 5. Character table of the symmetric group S_4.

Table 6. GCCI's of all the irreducible representations of S_4.

Table 7. GCCI's of $S_2[S_4]$ obtained from the GCCI's of S_2 and S_4.

Table 8. Character table of $S_2[S_4]$ obtained from the GCCI's in table 7 and the methods in reference

TABLE 1

C_3	E	(123)	(132)
order	1	1	1
A_1	1	1	1
E γ_1	1	ω	ω^*
E γ_2	1	ω^*	ω

$\omega = \exp(2\Pi i/3)$

TABLE 2

Γ	$3P^{\Gamma}$
A_1	$x_1^3 + 2x_3$
γ_1	$x_1^3 + (\omega + \omega^*)\ x_3$
γ_2	$x_1^3 + (\omega^* + \omega)\ x_3$
E	$2x_1^3 - 2x_3$

TABLE 3

No.	Γ	$18\, P^{\Gamma}$
1.	$(A_1 \# A_1) \otimes [2]'$	$x_1^6 + 4x_1^3 x_3 + 4x_3^2 + 3x_2^3 + 6x_6$
2.	$(A_1 \# A_1) \otimes [1^2]'$	$x_1^6 + 4x_1^3 x_3 + 4x_3^2 - 3x_2^3 - 6x_6$
3.	$\begin{Bmatrix} (\gamma_1 \# \gamma_1) \\ (\gamma_2 \# \gamma_2) \end{Bmatrix} \otimes [2]'$	$\begin{cases} x_1^6 + (\omega+\omega^*)^2 x_3^2 + 2(\omega+\omega^*)x_1^3 x_3 + 3x_2^3 + 3(\omega+\omega^*)x_6 \\ x_1^6 + (\omega^*+\omega)^2 x_3^2 + 2(\omega^*+\omega)x_1^3 x_3 + 3x_2^3 + 3(\omega^*+\omega)x_6 \end{cases}$
4.	$\begin{Bmatrix} (\gamma_1 \# \gamma_1) \\ (\gamma_2 \# \gamma_2) \end{Bmatrix} \otimes [1^2]'$	$\begin{cases} x_1^6 + (\omega+\omega^*)^2 x_3^2 + 2(\omega+\omega^*)x_1^3 x_3 - 3x_2^3 - 3(\omega+\omega^*)x_6 \\ x_1^6 + (\omega^*+\omega)^2 x_3^2 + 2(\omega^*+\omega)x_1^3 x_3 - 3x_2^3 - 3(\omega^*+\omega)x_6 \end{cases}$
5.	$(\gamma_1 \# \gamma_2) \uparrow C_2[C_3]$	$2x_1^6 - 4x_1^3 x_3 + 2x_3^2$
6.	$(A_1 \# E) \uparrow C_2[C_3]$	$4x_1^6 + 4x_1^3 x_3 - 8x_3^2$ OR $\begin{cases} 2x_1^6 - 2(\omega+\omega^*)x_1^3 x_3 - 2x_3^2 + 2(\omega+\omega^*)x_3^2 \\ 2x_1^6 - 2(\omega^*+\omega)x_1^3 x_3 - 2x_3^2 + 2(\omega^*+\omega)x_3^2 \end{cases}$

TABLE 4

$C_2[C_3]$	E	(123)	(132)	(123)(456)	(132)(465)	(132)(456)	(14)(25)(36)	(143625)	(142536)
Order	1	2	2	1	1	2	3	3	3
Γ_1	1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	1	1	-1	-1	-1
Γ_3	1	ω	ω^*	ω	ω^*	1	1	ω	ω^*
	1	ω^*	ω	ω^*	ω	1	1	ω^*	ω
Γ_4	1	ω	ω^*	ω	ω^*	1	-1	ω	ω^*
	1	ω^*	ω	ω^*	ω	1	-1	ω^*	ω
Γ_5	2	-1	-1	2	2	-1	0	0	0
Γ_6	2	$-\omega$	$-\omega^*$	2ω	$2\omega^*$	-1	0	0	0
	2	$-\omega^*$	$-\omega$	$2\omega^*$	2ω	-1	0	0	0

TABLE 5

S_4	E	(12)	(123)	(1234)	(12)(34)
Order	1	6	8	6	3
[4]	1	1	1	1	1
[31]	3	1	0	-1	-1
$[2^2]$	2	0	-1	0	2
$[21^2]$	3	-1	0	1	-1
$[1^4]$	1	-1	1	-1	1

TABLE 6

Γ	$24\ P^{\Gamma}$
[4]	$x_1^4 + 6x_1^2 x_2 + 8x_1x_3 + 6x_4 + 3x_2^2$
$[1^4]$	$x_1^4 - 6x_1^2 x_2 + 8x_1x_3 - 6x_4 + 3x_2^2$
[31]	$3x_1^4 + 6x_1^2 x_2 - 6x_4 - 3x_2^2$
$[21^2]$	$3x_1^4 - 6x_1^2 x_2 + 6x_4 - 3x_2^2$
$[2^2]$	$2x_1^4 - 8x_1x_3 + 2x_2^2$

TABLE 7

Γ	$1152\ P^{\Gamma}$
$([4]\#[4]) \otimes [2]'$	$x_1^8 + 12x_1^6 x_2 + 16x_1^5 x_3 + 12x_1^4 x_4 + 42x_1^4 x_2^2 + 36x_1^2 x_2^3 + 96x_1^3 x_2 x_3 + 72x_1^2 x_2 x_4 + 64x_1^2 x_3^2 + 48x_1 x_2^2 x_3 + 96x_1 x_3 x_4 + 144x_8 + 108x_4^2 + 180x_2^2 x_4 + 192x_2 x_6 + 36x_2^4$
$([4]\#[4]) \otimes [1^2]'$	$x_1^8 + 12x_1^6 x_2 + 16x_1^5 x_3 + 12x_1^4 x_4 + 42x_1^4 x_2^2 + 36x_1^2 x_2^3 + 96x_1^3 x_2 x_3 + 72x_1^2 x_2 x_4 + 64x_1^2 x_3^2 + 48x_1 x_2^2 x_3 + 96x_1 x_3 x_4 - 144x_8 - 36x_4^2 - 102x_2^2 x_4 - 192x_2 x_6 - 15x_2^4$
$([4]\#[31])\uparrow S_2[S_4]$	$6x_1^8 + 48x_1^6 x_2 + 48x_1^5 x_3 + 24x_1^4 x_4 + 84x_1^4 x_2^2 + 96x_1^3 x_2 x_3 - 48x_1 x_2^2 x_3 - 96x_1 x_3 x_4 - 72x_4^2 - 72x_2^2 x_4 - 18x_2^4$
$([4]\#[2^2])\uparrow S_2[S_4]$	$4x_1^8 + 24x_1^6 x_2 + 16x_1^5 x_3 + 24x_1^4 x_4 + 24x_1^4 x_2^2 + + 72x_1^2 x_2^3 - 96x_1^3 x_2 x_3 - 128x_1^2 x_3^2 + 48x_1 x_2^2 x_3 - 96x_1 x_3 x_4 + 72x_2^2 x_4 + 36x_2^4$
$([4]\#[21^2])\uparrow S_2[S_4]$	$6x_1^8 + 24x_1^6 x_2 + 48x_1^5 x_3 - 60x_1^4 x_2^2 + 48x_1^4 x_4 - 72x_1^2 x_2^3 - 96x_1^3 x_2 x_3 - 48x_1 x_2^2 x_3 + 96x_1 x_3 x_4 + 72x_1^4 x_4 - 18x_2^4$
$([4]\#[1^4])\uparrow S_2[S_4]$	$2x_1^8 + 32x_1^5 x_3 - 60x_1^4 x_2^2 - 144x_1^2 x_2 x_4 + 128x_1^2 x_3^2 + 96x_1 x_2^2 x_3 - 72x_4^2 + 18x_2^4$
$([31]\#[31]) \otimes [2]'$	$9x_1^8 + 36x_1^6 x_2 - 36x_1^4 x_4 + 18x_1^4 x_2^2 - 36x_1^2 x_2^3 - 72x_1^2 x_2 x_4 - 144x_8 - 36x_4^2 + 180x_2^2 x_4 + 81x_2^4$
$([31]\#[31]) \otimes [1^2]$	$9x_1^8 + 36x_1^6 x_2 - 36x_1^4 x_4 + 18x_1^4 x_2^2 - 36x_1^2 x_2^3 - 72x_1^2 x_2 x_4 + 144x_8 + 108x_4^2 - 108x_2^2 x_4 - 63x_2^4$

TABLE 7 (CONT.)

Γ	$1152\ P^{\Gamma}$
$([31]\#[2^2])\uparrow S_2[S_4]$	$12x_1^8 + 24x_1^6 x_2 - 48x_1^5 x_3 - 24x_1^4 x_4 + 24x_1^2 x_2^2 + 72x_1^2 x_2^3 - 96x_1^3 x_2 x_3 + 48x_1 x_2^2 x_3 + 96x_1 x_3 x_4 - 72x_2^2 x_4 - 18x_2^4$
$([31]\#[21^2])\uparrow S_2[S_4]$	$18x_1^8 - 108x_1^4 x_2^2 + 144x_1^2 x_2 x_4 - 72x_4^2 + 18x_2^4$
$([31]\#[1^4])\uparrow S_2[S_4]$	$6x_1^8 - 24x_1^6 x_2 + 48x_1^5 x_3 - 48x_1^4 x_4 - 60x_1^4 x_2^2 + 72x_1^2 x_2^3 + 96x_1^2 x_2 x_3 - 48x_1 x_2^2 x_3 - 96x_1 x_3 x_4 + 72x_4^2 - 18x_2^4$
$([2^2]\#[2^2]) \otimes [2]'$	$4x_1^8 - 32x_1^5 x_3 + 24x_1^4 x_2^2 + 64x_1^2 x_3^2 - 96x_1 x_3 x_2^2 + 144x_4^2 - 192x_2 x_6 + 84x_2^4$
$([2^2]\#[2^2]) \otimes [1^2]'$	$4x_1^8 - 32x_1^5 x_3 + 24x_1^4 x_2^2 + 64x_1^2 x_3^2 - 96x_1 x_3 x_2^2 - 144x_4^2 + 192x_2 x_6 - 12x_2^4$
$([2^2]\#[21^2])\uparrow S_2[S_4]$	$12x_1^8 - 24x_1^6 x_2 - 48x_1^5 x_3 + 24x_1^4 x_4 + 36x_1^4 x_2^2 - 72x_1^2 x_2^3 + 96x_1^3 x_2 x_3 + 48x_1 x_2^2 x_3 - 96x_1 x_3 x_4 + 72x_2^2 x_4 - 36x_2^4$
$([2^2]\#[1^4])\uparrow S_2[S_4]$	$4x_1^8 - 24x_1^6 x_2 + 16x_1^5 x_3 - 24x_1^4 x_4 + 24x_1^4 x_2^2 - 72x_1^2 x_2^3 + 96x_1^3 x_2 x_3 - 128x_1^2 x_3^2 + 48x_1 x_2^2 x_3 + 96x_1 x_3 x_4 - 72x_2^2 x_4 + 36x_2^4$
$([21^2]\#[21^2]) \otimes [2]'$	$9x_1^8 - 36x_1^6 x_2 + 36x_1^4 x_4 + 18x_1^4 x_2^2 + 36x_1^2 x_2^3 - 72x_1^2 x_2 x_4 + 144x_8 - 36x_4^2 - 180x_2^2 x_4 + 81x_2^4$
$([21^2]\#[21^2]) \otimes [1^2]'$	$9x_1^8 - 36x_1^6 x_2 + 36x_1^4 x_4 + 18x_1^4 x_2^2 + 36x_1^2 x_2^3 - 72x_1^2 x_2 x_4 - 144x_8 + 108x_4^2 + 108x_2^2 x_4 - 63x_2^4$

TABLE 7 (CONT.)

Γ	$1152\ P^{\Gamma}$
$([21^2]\#[1^4])\uparrow S_2[S_4]$	$6x_1^8 - 48x_1^6x_2 + 48x_1^5x_3 - 24x_1^4x_4 + 84x_1^4x_2^2 - 96x_1^3x_2x_3 - 48x_1x_2^2x_3 + 96x_1x_3x_4 - 72x_4^2 + 72x_2^2x_4 - 18x_2^4$
$([1^4]\#[1^4]) \otimes [2]'$	$x_1^8 - 12x_1^6x_2 + 16x_1^5x_3 - 12x_1^4x_4 + 42x_1^4x_2^2 - 36x_1^2x_2^3 - 96x_1^3x_2x_3 + 72x_1^2x_2x_4 + 64x_1^2x_3^2 + 48x_1x_2^2x_3 - 96x_1x_3x_4 - 144x_8 + 108x_4^2 - 180x_2^2x_4 + 192x_2x_6 + 33x_2^4$
$([1^4]\#[1^4]) \otimes [1^2]'$	$x_1^8 - 12x_1^6x_2 + 16x_1^5x_3 - 12x_1^4x_4 + 42x_1^4x_2^2 - 36x_1^2x_2^3 - 96x_1^3x_2x_3 + 72x_1^2x_2x_4 + 64x_1^2x_3^2 + 48x_1x_2^2x_3 - 96x_1x_3x_4 + 144x_8 - 36x_4^2 + 108x_2^2x_4 - 192x_2x_6 - 15x_2^4$

TABLE 8

$S_2[S_4]$	E	(12)	(123)	(1234)	(12)(34)	(12)(56)	(12)(34)(56)	(12)(567)	(12)(5678)	(123)(567)	(234)(56)(78)	(234)(5678)	(18273645)	(1234)(5678)	(1825)(3647)	(12)(34)(5678)	(1825)(37)(46)	(15)(273648)	(12)(34)(56)(78)	(15)(28)(37)(46)
Order	1	12	16	12	6	36	36	96	72	64	48	96	144	36	72	36	144	192	9	24
Γ_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
Γ_3	6	4	3	2	2	2	0	1	0	0	-1	-1	0	-2	0	-2	0	0	-2	0
Γ_4	4	2	1	2	4	0	2	-1	0	-2	1	-1	0	0	0	2	0	0	4	0
Γ_5	6	2	3	4	2	-2	-2	-1	0	0	-1	1	0	2	0	0	0	0	-2	0
Γ_6	2	0	2	0	2	-2	0	0	-2	2	2	0	0	-2	0	0	0	0	2	0
Γ_7	9	3	0	-3	-3	1	-1	0	-1	0	0	0	-1	1	-1	1	1	0	1	+3
Γ_8	9	3	0	-3	-3	1	-1	0	-1	0	0	0	+1	1	1	1	-1	0	1	-3
Γ_9	12	2	-3	-2	4	0	2	-1	0	0	1	1	0	0	0	-2	0	0	-4	0
Γ_{10}	18	0	0	0	-6	-2	0	0	2	0	0	0	0	-2	0	0	0	0	2	0
Γ_{11}	6	-2	3	-4	2	-2	2	1	0	0	-1	-1	0	2	0	0	0	0	-2	0
Γ_{12}	4	0	-2	0	4	0	0	0	0	1	-2	0	0	0	+2	0	0	-1	4	2
Γ_{13}	4	0	-2	0	4	0	0	0	0	1	-2	0	0	0	-2	0	0	1	4	-2
Γ_{14}	12	-2	-3	2	4	0	-2	1	0	0	1	-1	0	0	0	2	0	0	-4	0

TABLE 8 CONT.

	E	(12)	(123)	(1234)	(12)(34)	(12)(56)	(12)(34)(56)	(12)(567)	(12)(5678)	(123)(567)	(234)(56)(78)	(234)(5678)	(18273645)	(1234)(5678)	(1825)(3647)	(12)(34)(5678)	(1825)(37)(46)	(15)(273648)	(12)(34)(56)(78)	(15)(28)(37)(46)
Order	1	12	16	12	6	36	36	96	72	64	48	96	144	36	72	36	144	192	9	24
Γ_{15}	4	-2	1	-2	4	0	-2	+1	0	-2	1	1	0	0	0	-2	0	0	4	0
Γ_{16}	9	-3	0	3	-3	1	1	0	-1	0	0	0	1	+1	-1	-1	-1	0	1	3
Γ_{17}	9	-3	0	3	-3	1	1	0	-1	0	0	0	-1	1	1	-1	1	0	+1	-3
Γ_{18}	6	-4	3	-2	2	2	0	-1	0	0	-1	1	0	-2	0	2	0	0	-2	0
Γ_{19}	1	-1	1	-1	1	1	-1	-1	1	1	1	-1	-1	1	1	-1	-1	1	1	1
Γ_{20}	1	-1	1	-1	1	1	-1	-1	1	1	1	-1	1	1	-1	-1	1	-1	1	-1

Table 9. The GCCI's of the group $S_2[S_2]$

Γ	$8 \cdot P_G^{\chi}$
A_1	$x_1^4 + 2x_1^2x_2 + 3x_2^2 + 2x_4$
A_2	$x_1^4 - 2x_1^2x_2 - x_2^2 + 2x_4$
B_1	$x_1^4 + 2x_1^2x_2 - x_2^2 - 2x_4$
B_2	$x_1^4 - 2x_1^2x_2 + 3x_2^2 - 2x_4$
E	$2x_1^4 - 2x_2^2$

Table 10. Generalized isomer enumeration of substituted hydrazine. The set of functions from the set of vertices to substituents with the weight a^2b^2, the patterns (isomers) and the irreducible representations contained in each pattern are shown below.

Functions	Pattern	Irreducible Representations
aa bb bb aa	aa bb	$A_1 \oplus B_1$
ab ab ab ba ba ab ba ba	ab ab	$A_1 \oplus B_2 \oplus E$