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Generators of the character tables of generalized wreath product groups

K. Balasubramanian*

Department of Chemistry, Arizona State University, Tempe, AZ 85287-1604, USA

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Summary. A method based on the cycle-type matrix algebra is devised to generate the character tables of generalized wreath products which are useful in describing the symmetry groups of non-rigid molecules, NMR groups, groups of non-rigid van der Waals complexes, the groups of space types in configuration interaction calculations, etc. This newly developed method is illustrated with examples.

Key words: Non-rigid molecules – Generalized wreath products – Character tables

1. Introduction

It is now well-recognized that the symmetry groups of non-rigid molecules [1, 2], NMR groups [3], groups of weakly-bound van der Waals complexes [9], configuration symmetry groups [4, 5] for isomer enumeration and isomerization reactions [6–8], symmetry groups in configuration interaction calculations [10], symmetry groups of crystals exhibiting distortions [2] and the symmetry groups of many chemical graphs [11–13], can be expressed as generalized wreath products. Some groups related to the topic of chirality polynomials are also expressible as wreath products [14]. The order of these groups rises both factorially and exponentially and thus the computation of character tables for these groups could be difficult. For example, the symmetry group of the non-rigid benzene trimer contains 20 736 permutations. This simple example illustrates the computational complexity of the task of evaluating characters of wreath product groups and generalized wreath product groups. It is of interest to note that the related topological groups (automorphism groups) of graphs are also useful in several applications [16–18]. The generalized wreath product algebra is useful in the operator method formulation of NMR [19, 20]. For a review of this topic see [4].

* Camille and Henry Dreyfus Teacher-Scholar

While rigorous techniques have been developed to compute the generalized character cycle indices (GCCI) of generalized wreath product groups [4, 19, 20], this is not the case for the computation of the actual character tables. Recently, Liu and the present author [22] have developed a computer code for efficient calculation of the character cycle indices. Such cycle indices are quite useful for computing nuclear spin statistics, enumeration of isomers, spin functions and in computing chirality polynomials. However, it is necessary to have the actual character tables for applications such as the prediction of allowed transitions, the classification of wave functions, and the determination of vibrational selection rules. The objective of the present paper is to develop a new cycle type matrix algebraic method for the generation of character tables of generalized wreath products. Section 2 outlines preliminaries pertaining to generalized wreath product groups. Section 3 describes the cycle type matrix algebra. Section 4 shows how to use the matrix algebraic method to obtain the character table of a non-rigid tetraphenyl.

2. Mathematical preliminaries pertaining to generalized wreath product groups

We start with an illustration of the wreath product group using the hydrazine molecule within a particles–in–a–box model [2]. Figure 1 shows the particles–in–a–box permutations in the non-rigid molecular group of hydrazine. Let the protons of the first nitrogen atom (A) be labeled 1 and 2 while the protons of the second nitrogen (B) be labeled 3 and 4. The permutations in the wreath product $S_2[S_2]$ can be visualized using a particles–in–a–box model as shown in Fig. 1. Let us associate boxes A and B with the nitrogen atoms A and B, respectively. Let the protons 1 and 2 be particles in the box A and the protons 3 and 4 be particles in the box B. Suppose G is a permutation groups of boxes, which is S_2 for hydrazine in Fig. 1, comprising permutations {(A)(B),(AB)}. Let H be the

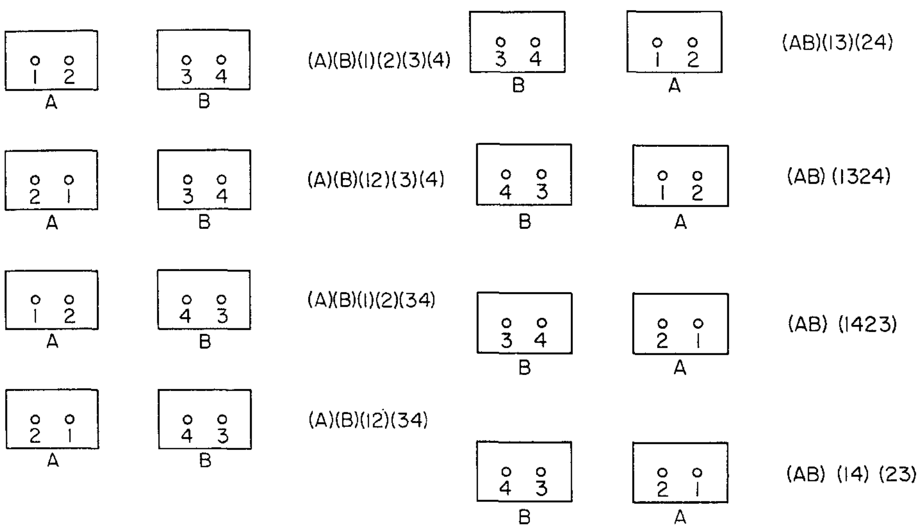

Fig. 1. Particles–in–a–box model of hydrazine

group acting on particles within the various boxes. In this example, H is the group of the permutations of the particles in the boxes, namely, the S_2 group. Then the wreath product of G with H, denoted by $G[H]$ contains permutations of both boxes, particles and the permutations of particles induced by the permutations of boxes. As seen from Fig. 1, a permutation of boxes in turn induces a permutation of the particles. A simple permutation of boxes A and B in Fig. 1, without permuting the particles individually in each box, induces an overall permutation of (AB)(13)(24). Given the group G of boxes and the group H of particles in each box, the overall group of all particles in all boxes is the wreath product of G with H, denoted $G[H]$. If there are n boxes, the number of elements in this group can be seen to be $|G||H|^n$, where $|G|$ is the number of elements in the group G and $|H|$ is the number of elements in the group H. Figure 1 illustrates the possible permutations in the wreath product $S_2[S_2]$. The non-rigid molecular group of biphenyl is also isomorphic with $S_2[S_2]$. The wreath product $S_2[S_3]$, which is the NMR group of ethane and the group of the ammonia dimer, consists of $6^2 \cdot 2 = 72$ permutations, while $S_2[S_2]$ contains eight permutations. For mathematical details on wreath products see [23].

A formal definition of the wreath product group can be given. Suppose $\Omega = \{1, 2, \ldots, n\}$ is a set of elements (boxes). Let G be a permutation group acting on Ω. Let H be another permutation group acting on particles within boxes. The set $\{(g; \pi) \mid \pi: \Omega \to H, g \in G\}$ spans the wreath product group $G[H]$. The product of two elements $(g; \pi)$ and $(g'; \pi')$ is defined as [23]

$$(g; \pi)(g'; \pi') = (gg'; \pi\pi'_g), \tag{1}$$

where

$$\pi'_g(i) = \pi'(g^{-1}i), \quad \forall i \in \Omega. \tag{2}$$

The product of two maps $\pi, \pi': \Omega \to H$ is defined as

$$\pi\pi'(i) = \pi(i)\pi'(i), \quad \forall i \in \Omega. \tag{3}$$

The element $(e; e')$ is the identity where $e \in G$, and e' is the identity map defined by

$$e'(i) = {}^1H, \quad \forall i \in \Omega, \tag{4}$$

where ${}^1H$ is the identity element for the group H. The inverse of $(g; \pi)$ is $(g^{-1}; \pi_{g^{-1}})$.

The generalization of the wreath product $G[H]$ to a generalized wreath product group $G[H_1, H_2, \ldots, H_n]$ [1, 2, 4] becomes necessary when the number of particles in different boxes is not the same. Linear tetraphenyl (Fig. 2) is an example: rotation around the bond connecting the phenyl rings is freely allowed, and the terminal rings are not equivalent to the non-terminal rings, so, generalization of the wreath product group to the generalized wreath product group becomes necesssary. In this case, the set $\Omega = \{1, 2, 3, 4\}$ of the boxes is partitioned into two sets $Y_1 = \{1, 4\}$ and $Y_2 = \{2, 3\}$ so that all the boxes in a given set Y_i are equivalent. In this setup a mathematical definition of generalized wreath product is as follows:

Suppose a set $\Omega = \{1, 2, \ldots, n\}$ is partitioned into mutually disjoint sets $Y_1, Y_2, \ldots, Y_t$. Let G be a permutation group acting on Ω such that all its cycles are contained within the same Y_i 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 $(i = 1, 2, \ldots, t)$. The set

$$\{(g; \pi_1, \pi_2, \ldots, \pi_t) \mid g \in G, \pi_i: Y_i \to H_i\} \tag{5}$$

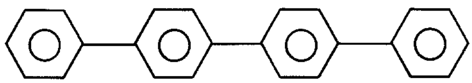

Fig. 2. A non-rigid tetraphenyl molecule. The permutation subgroup of the symmetry group of this molecule is the generalized wreath product $S_2[S_2, S_2]$. For its conjugacy classes and character tables see Tables 2 and 3

is called the generalized wreath product group. Each element in the generalized wreath product group can also be represented by an ordered $(t+1)$-tuple of the form

$$(g; h_{11}, h_{12}, \ldots, h_{1m_1}; h_{21}, h_{22}, \ldots, h_{2m_2}; \ldots; h_{t1}, h_{t2}, \ldots, h_{tm_t}), \quad \text{where } m_i = |Y_i|, \tag{6}$$

$g \in G$, and $h_{ij} \in H_i$. It can be seen that the generalized wreath product set forms a group and it is denoted $G[H_1, H_2, \ldots, H_t]$. For the example in Fig. 2, the generalized wreath product group is simply $S_2[S_2, S_2]$, which contains $2 \cdot 2^2 \cdot 2^2 = 32$ elements. The group G in this case is S_2 and contains the permutations $\{(1)(2)(3)(4), (14)(23)\}$. T_i is simply the set of particles in each box.

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 by dividing the set $\Delta = \{1, 2, \ldots, n\prod_{i=1}^{t} t_i\}$ into disjoint subsets $\Delta_{11}, \Delta_{12}, \ldots, \Delta_{1m_1}, \Delta_{21}, \Delta_{22}, \ldots, \Delta_{2m_2}, \ldots, \Delta_{t1}, \Delta_{t2}, \ldots, \Delta_{tm_t}$. Subsequently, for a given i, the direct product of the group H_{ij} acting on Δ_{ij} is obtained by varying j from 1 to m_i. In this setup, the permutational representation of the generalized wreath product is obtained as

$$\begin{aligned} G[H_1, H_2, \ldots, H_t] = [(&H_{11} \times H_{12} \times \cdots \times H_{1m_1}) \\ &\times (H_{21} \times H_{22} \times \cdots \times H_{2m_2}) \\ &\times \cdots \times (H_{t1} \times \cdots \times H_{tm_t})] \cdot G', \end{aligned} \tag{7}$$

where

$$G' = \{(g; e_1, e_2, \ldots, e_t) \,|\, g \in G, e_i(j) = {}^1H_i \text{ (the identity of the group } H_i), j \in Y_i\} \tag{8}$$

and H_{ij} is a copy of the group H_i. The product $[(H_{11} \times H_{12} \times \cdots \times H_{1m_1}) \times (H_{21} \times H_{22} \times \cdots \times H_{2m_2}) \times \cdots \times (H_{t1} \times H_{t2} \times \cdots \times H_{tm_t})]$, denoted by $H_1^{m_1^*} \times H_2^{m_2^*} \times \cdots \times H_t^{m_t^*}$, is called the basis group of $G[H_1, H_2, \ldots, H_t]$.

Although the representation theory of generalized wreath products is described in adequate details in [1], the most important points are given below. These are required for the further development of cycle type matrix algebra.

Let the irreducible representation of $H_1^{m_1^*} \times H_2^{m_2^*} \times \cdots \times H_t^{m_t^*}$ be denoted $\Gamma = F_1^{m_1^*} \# F_2^{m_2^*} \# \cdots \# F_t^{m_t^*}$, where $F_i^{m_i^*}$ is the outer tensor product $F_{i1} \# F_{i2} \# F_{i3} \# \cdots \# F_{im_1}$; 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 $\#_i F'^{m_i^*}_i$ 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

$$g(\#_i F_i^{m_i^*}) = \#_i F'^{m_i^*}_i. \tag{9}$$

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 consists of the set of permutations satisfying the following property:

$$G_\Gamma[H_1, H_2, \ldots, H_t] = \{(g; \pi_1, \pi_2, \ldots, \pi_t) \,|\, \Gamma(g'; \pi_1, \pi_2, \ldots, \pi_t) \sim \Gamma\}, \quad (10)$$

where $\Gamma = \#_i F_i^{m_i^*}$. A permutation representation of the inertia group $G_\Gamma[H_1, H_2, \ldots, H_t]$ is $(H_1^{m_1^*} \times H_2^{m_2^*} \times \cdots \times H_t^{m_t^*}) \cdot G'_\Gamma$ where G'_Γ is known as the inertia factor. The irreducible representations of $G[H_1, H_2, \ldots, H_t]$ are given by the representations induced by $\Gamma \otimes F'_\Gamma$ (F'_Γ is an irreducible representation of the inertia factor group G'_Γ). Symbolically, $(\#_i F_i^{m_i^*} \otimes F'_\Gamma) \uparrow G(H_1, H_2, \ldots, H_t)$ are the irreducible representations of $G[H_1, H_2, \ldots, H_t]$.

For a given irreducible representation, $\#_i F_i^{m_i^*}$, its inertia factor group G'_Γ, i.e., the quotient group of the inertia group $G'_\Gamma[H_1, H_2, \ldots, H_t]$, can be seen to be a subgroup of G.

The generalized character cycle index (GCCI) of an irreducible representation Γ of a group G whose character is χ is given by [15, 19–21]

$$P_G^\chi = \frac{1}{|G|} \sum_{g \in G} \chi(g) s_1^{b_1} s_2^{b_2} \cdots s_n^{b_n}, \quad (11)$$

where the sum is over all the elements g of the group G, $|G|$ is the number of elements in G, and $s_1^{b_1} s_2^{b_2} \cdots s_n^{b_n}$ is a cycle representation of a permutation $g \in G$ if it generates b_1 cycles of length 1, b_2 cycles of length 2 ... and b_n cycles of length n.

If G'_Γ is the inertia group corresponding to the irreducible representation Γ, then G'_Γ can be seen to divide the set of Ω into disjoint sets $Y_1, Y_2, \ldots, Y_l$. Note that this partitioning is identical to $Y_1, Y_2, \ldots, Y_t$ when $G'_\Gamma = G$. This is accomplished by taking the permutations of G'_Γ and applying them to Ω. The cycle index of G'_Γ, which corresponds to the representation F'_Γ with character χ of G'_Γ, is defined with two-index dummy variable s_{ij} as

$$p_{G'_\Gamma}^\chi = \frac{1}{|P_{G'_\Gamma}^\chi|} = \sum_{g \in G} \chi(g) \prod_i \prod_j s_{ij}^{c_{ij}(g)}, \quad (12)$$

where $c_{ij}(g)$ denotes the number of j-cycles of g in the set Y_i, and $\chi(g)$ is the character corresponding to the element g in the irreducible representation F'_Γ of G'_Γ. Let $Z_i(s_1, s_2, \ldots)$ denote the GCCI of the irreducible representation made of $\#_i F_i^{m_i^*}$. Define Z_{ij} as

$$Z_{ij} = Z_i(s_k \to s_{kj}), \quad (13)$$

where the symbol $s_k \to s_{kj}$ stands for the operation of replacing every cycle of length k by a cycle of length kj (kj denotes the product of k and j).

The generalized character cycle index of the irreducible representation $\#_i F_i^{m_i^*} \otimes F'_\Gamma \uparrow G[H_1, H_2, \ldots, H_n]$ is given by [15, 19, 20]

$$P_{G'_\Gamma}^\chi(s_{ij} \to Z_{ij}). \quad (14)$$

Thus, the generalized character cycle index of the irreducible representation is obtained by replacing every s_{ij} in $P_{G'_\Gamma}^\chi$ by the cycle index Z_{ij}.

The above result can be illustrated by the example of the non-rigid tetraphenyl molecule in Fig. 2. The set $\Omega = \{1, 2, 3, 4\}$, where the elements 1 and 4 are terminal rings and 2 and 3 are the non-terminal rings, is partitioned into sets $Y_1 = \{1, 4\}$ and $Y_2 = \{2, 3\}$ for the case where the inertia factor is the whole group G. Consider the irreducible representation $[1^2]\#[2]\#[2]\#[1^2]\otimes[1^2]'$ as an example. The inertia factor group for $[1^2]\#[2]\#[2]\#[1^2]$ is the whole group

S_2. The GCCI of the $[1^2]'$ representation of S_2 is given by

$$P_{S_2}^{[1^2]'} = \tfrac{1}{2}[s_{11}^2 s_{21}^2 - s_{12}s_{22}]. \tag{15}$$

The indices Z_{11}, Z_{21}, Z_{12} and Z_{22} for the protons of tetraphenyl are given by

$$Z_{11} = \tfrac{1}{2}[s_1^5 - s_1 s_2^2], \tag{16}$$

$$Z_{12} = \tfrac{1}{2}[s_2^5 - s_2 s_4^2], \tag{17}$$

$$Z_{21} = \tfrac{1}{2}[s_1^4 + s_2^2], \tag{18}$$

$$Z_{22} = \tfrac{1}{2}[s_2^4 + s_4^2]. \tag{19}$$

Thus for $\Gamma = [1^2]\#[2]\#[2]\#[1^2]\otimes[1^2]'$

$$P_{S_2}^{\Gamma} = P_{S_2}^{[1^2]'}(s_{ij} \to Z_{ij}) \tag{20}$$

$$= \tfrac{1}{2}[\{\tfrac{1}{2}(s_1^5 - s_1 s_2^2)\}^2\{\tfrac{1}{2}(s_1^4 + s_2^2)\}^2 - \tfrac{1}{2}(s_2^5 - s_2 s_4^2)\,\tfrac{1}{2}(s_2^4 + s_4^2)] \tag{21}$$

$$= \tfrac{1}{32}[s_1^{18} - 2s_1^{14}s_2^2 + s_1^{10}s_2^4 + 2s_1^{14}s_2^2 - 4s_1^{10}s_2^4$$
$$+ 2s_1^6 s_2^6 + s_1^{10}s_2^4 - 2s_1^6 s_2^6 + s_1^2 s_2^8 - 4s_2^9 + 4s_2 s_4^4]. \tag{22}$$

Consequently, the GCCI of the irreducible representation $[1^2]\#[2]\#[2]\#[1^2]\otimes[1^2]'$ of the $S_2[S_2, S_2]$ group is simply generated from the GCCIs of S_2.

Although the GCCIs obtained above are useful in several chemical physics applications such as NMR, nuclear spin statistics, isomer enumeration, molecular spectroscopy, etc., they do not always generate the complete character. This is because two different conjugacy classes can have the same cycle representation. A trivial example is the rotational subgroup C_3 for which the c_3 and c_3^2 operations have the same cycle representations s_3 but do not belong to the same conjugacy class. Thus in general one needs more powerful algebraic methods to generate characters.

3. The cycle type matrix algebra for character generators

The cycle type matrix algebraic method described below is useful for computing the characters of the generalized wreath product group $G[H_1, H_2, \ldots, H_n]$, if G happens to be isomorphic with S_n containing $n!$ permutations of n boxes. For the special case of the wreath product $S_n[H]$, a cycle type matrix [23] can be obtained that has one-to-one correspondence with a conjugacy class of $S_n[H]$. Let $g \in G$ generate a_1 cycles of length 1, a_2 cycles of length 2, etc. Equivalently, the cycle type of $g \in G$, T_g is $(a_1, a_2, \ldots, a_n)$. Suppose $c_1, c_2, \ldots, c_s$ are the conjugacy classes of the group H. Suppose a_{ik} of these cycle products belong to c_i, then a simple $s \times n$ matrix, which is called the cycle type matrix for an element $(g; \pi)$ of the wreath product, is shown below:

$$T(g; \pi) = a_{ik} \quad (1 \leqslant i \leqslant s) \quad (1 \leqslant k \leqslant n). \tag{23}$$

We now illustrate the above formalism with the example of the $S_3[S_3]$ group. Consider the conjugacy class $\{(1)(2)(3); (123), (123), (123)\}$ of this group. This permutation is isomorphic with (123)(456)(789). The cycle type matrix for this permutation is shown below:

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 3 & 0 & 0 \end{bmatrix}, \tag{24}$$

A simple interpretation of the cycle type matrix is

$$\begin{bmatrix} s_1^3 & s_2^3 & s_3^3 \\ s_1 s_2 & s_2 s_4 & s_3 s_6 \\ s_3 & s_6 & s_9 \end{bmatrix}. \tag{25}$$

The first column represents the cycle types generated in the group H if $g \in G$ is the identity, the second column represents the possible cycle types generated by replacing every $s_1^{b_1} s_2^{b_2} \cdots s_k^{b_k}$ in the first column by $s_2^{b_1} s_4^{b_2} \cdots s_{2k}^{b_k}$, while the third column represents the possible cycle types obtained by replacing every $s_1^{b_1} s_2^{b_2} \cdots s_k^{b_k}$ by $s_3^{b_1} s_6^{b_2} \cdots s_{3k}^{b_k}$. Since in the element $\{(1)(2)(3); (123), (123), (123)\}$, g is the identity, only the first column of the matrix can contain non-zero elements. Since all three H group elements have the same cycle types corresponding to the third row and first column, a_{31} is 3 and the rest of the elements are zero. Next consider $\{(12)(3); (123), 1, 1\} \in S_3[S_3]$. The element g has a cycle type $s_1 s_2$; thus, both first and second columns will contain non-zero elements. Since the first element in H belongs to the third conjugacy class while the other two belong to the first class, the cycle type matrix is

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \tag{26}$$

The resulting cycle type of $s_1^3 s_6$ can be easily verified as the correct cycle type for the above element. If in general a cycle type $s_1^{b_1} s_2^{b_2} \cdots s_n^{b_n}$ is obtained then

$$\sum_{k=1}^{n} k b_k = m, \tag{27}$$

where $m = |Y|^{|\Omega|}$.

The above example illustrates that, in terms of cycle type matrix algebra, the generalized wreath product substitution $S_k \to S_{kj}$ corresponds to moving the first column to the jth column of the matrix type. This is the key underlying principle we use to generate the characters. That is, although in general there is no one-to-one correspondence between the cycle type $s_1^{b_1} s_2^{b_2} \cdots s_n^{b_n}$ and the conjugacy class of $S_n[H]$, there is a one-to-one correspondence between the cycle type matrices and the conjugacy classes of $S_n[H]$. For example, the element $\{(123); 1, 1, 1\}$ and $\{1; (123), (123), (123)\}$ belong to different type conjugacy classes, but their cycle types are both s_3^3. However, the cycle type matrices of the former and latter elements differ and are shown below:

$$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 3 & 0 & 0 \end{bmatrix}. \tag{28}$$

Consequently, the cycle type matrix is a more powerful discriminator than the simple scalar cycle type $s_1^{b_1} s_2^{b_2} \cdots s_n^{b_n}$.

The generalized wreath product substitution $S_{ij} \to Z_{ij}$ described in Sect. 2 can be equivalently carried out using the cycle type matrices rather than using the cycle index polynomials. This provides a powerful general character generator for the groups $S_n[H_1, H_2, \ldots, H_n]$. This requires replacing the ordinary cycle index polynomials by a combination of cycle type matrices of $H_1, H_2, \ldots, H_n$, and subsequently replacing every s_{ij} in P_G^Γ by the appropriate matrix combination of cycle type matrices $T(M)_{ij}$. In symbols, suppose P_G^Γ is the GCCI of an irreducible representation Γ in G. Let $T(M)_{ij}$ be the appropriate combination of cycle type matrices obtained using the procedure described below. Then a new cycle type matrix of $G[H_1, H_2, \ldots, H_n]$ corresponding to the overall representation F^* of $G[H_1, H_2, \ldots, H_n]$ is obtained as

$$T[G(H_1, H_2, \ldots, H_n)]F^* = P_G^\Gamma(s_{ij} \to T(M)_{ij}). \tag{29}$$

Let us illustrate the above procedure with a simple example. Consider the representation $\Gamma_{13} = [1^2] \# [1^2] \# [1^2] \# [1^2] \otimes [2]'$ of the tetraphenyl in Fig. 2. The inertia factor group is the whole group S_2 for this representation. The cycle index $P_{S_2}^{[2]'}$ is given by

$$P_{S_2}^{[2]'} = \tfrac{1}{2}\,[s_{11}^2 s_{21}^2 + s_{12}s_{22}]. \tag{30}$$

The matrix types $T(M)_{ij}$ are given by

$$T(M)_{11} = T(M)_{21} = \frac{1}{2}\left\{\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix} \ominus \begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix}\right\}, \tag{31}$$

$$T(M)_{12} = T(M)_{22} = \frac{1}{2}\left\{\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix} \ominus \begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}\right\}. \tag{32}$$

(Note that in the above expression the $\ominus$ and $\oplus$ signs do not mean simple matrix subtraction or addition.) As we shall see below, only the coefficients are treated as scalars. The matrix elements are carefully manipulated in accordance with cycle types and no additions or subtractions of matrices are carried out in the ordinary sense. Hence the substitution $S_{ij} \to T(M)_{ij}$ yields

$$\begin{aligned}
T(\Gamma_{13}) = \frac{1}{36}\Bigg\{&\left(\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix} \ominus \begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix}\right)^2\left(\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix} \ominus \begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix}\right)^2\\
&+4\left(\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix} \ominus \begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}\right)\left(\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix} \ominus \begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}\right)\Bigg\}\\
= \frac{1}{36}\Bigg\{&\begin{bmatrix}2 & 0\\ 0 & 0\end{bmatrix}\begin{bmatrix}2 & 0\\ 0 & 0\end{bmatrix} \ominus 2\begin{bmatrix}1 & 0\\ 1 & 0\end{bmatrix}\begin{bmatrix}2 & 0\\ 0 & 0\end{bmatrix} \oplus \begin{bmatrix}0 & 0\\ 2 & 0\end{bmatrix}\begin{bmatrix}2 & 0\\ 0 & 0\end{bmatrix}\\
&\ominus 2\begin{bmatrix}2 & 0\\ 0 & 0\end{bmatrix}\begin{bmatrix}1 & 0\\ 1 & 0\end{bmatrix} \ominus 2\begin{bmatrix}0 & 0\\ 2 & 0\end{bmatrix}\begin{bmatrix}1 & 0\\ 1 & 0\end{bmatrix} \oplus 2\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix}\\
&\oplus 2\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix} \oplus \begin{bmatrix}2 & 0\\ 0 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\ 2 & 0\end{bmatrix} \ominus 2\begin{bmatrix}1 & 0\\ 1 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\ 2 & 0\end{bmatrix}\\
&\oplus \begin{bmatrix}0 & 0\\ 2 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\ 2 & 0\end{bmatrix} \oplus 4\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix}\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix}\\
&\ominus 4\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix} \ominus 4\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix} \oplus 4\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}\Bigg\}.
\end{aligned} \tag{33}$$

In simplifying the above expression, the fact that two cycle type matrices can be combined into only one matrix if they correspond to equivalent members of the same Y set is used. For the example in Fig. 2, the first and fourth rings are equivalent, and second and third rings are equivalent. Thus the matrices corresponding to the equivalent rings can be combined if they are the same. Consequently,

$$\text{(i)}\ \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}^2 = \begin{bmatrix}2 & 0\\0 & 0\end{bmatrix},$$

$$\text{(ii)}\ \begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}$$

is not equivalent to

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

but

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

and

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

are equivalent. This is because the group $G = S_2$ permutes the terminal phenyl rings simultaneously with the non-terminal phenyl rings. The coefficients in the above expression generate the character. The various cycle type matrices are the conjugacy classes of the generalized wreath product group $S_2[S_2, S_2]$. Consequently, the cycle type matrix algebra simultaneously generates the conjugacy classes and the characters.

4. Example of a non-rigid tetraphenyl

Consider the non-rigid tetraphenyl in Fig. 2 as an example. We shall use this example to illustrate the various techniques described above. The group G is S_2 while the total non-rigid permutation group is $S_2[S_2, S_2]$. (Note that the permutation-inversion group [24] is the direct product of the permutation and inversion group for this case.) The irreducible representations of basis groups, the inertia factor groups and the final irreducible representations are shown in Table 1. The conjugacy classes and the order of various conjugacy classes are shown in Table 2. The actual character table is obtained through repeated $s_{ij} \to T(M)_{ij}$ substitutions for each representation described and illustrated in Sect. 3. The character table is shown in Table 3.

As an additional illustration of the $s_{ij} \to T(M)_{ij}$ substitution we consider another example. Consider $\Gamma_4 = [2] \# [2] \# [2] \# [1^2] \uparrow S_2[S_2, S_2]$. The inertia factor is the identify group for this case. Hence

$$P^{\Gamma} = s_{11}^{(1)} s_{11}^{(2)} s_{21}^{(1)} s_{21}^{(2)}. \tag{34}$$

Table 1. Irreducible representations of $S_2[S_2, S_2]$, the generalized wreath product group of tetraphenyl in Fig. 1

Representation of the basis group, $H_1 \times H_2 \times H_3 \times H_4$	Inertia factor	Total representation	Dimension
$[2]\#[2]\#[2]\#[2]$	S'_2	$\Gamma_1 = [2]\#[2]\#[2]\#[2] \otimes [2]'$	1
		$\Gamma_2 = [2]\#[2]\#[2]\#[2] \otimes [1^2]'$	1
$[2]\#[2]\#[2]\#[1^2]$	E'	$\Gamma_3 = [2]\#[2]\#[2]\#[1^2] \otimes [1]' \uparrow S_2[S_2, S_2]$	2
$[2]\#[2]\#[1^2]\#[2]$	E'	$\Gamma_4 = [2]\#[2]\#[1^2]\#[2] \otimes [1]' \uparrow S_2[S_2, S_2]$	2
$[2]\#[2]\#[1^2]\#[1^2]$	E'	$\Gamma_5 = [2]\#[2]\#[1^2][1^2] \otimes [1]' \uparrow S_2[S_2, S_2]$	2
$[2]\#[1^2]\#[2]\#[1^2]$	E'	$\Gamma_6 = [2]\#[1^2]\#[2]\#[1^2] \otimes [1]' \uparrow S_2[S_2, S_2]$	2
$[2]\#[1^2]\#[1^2]\#[2]$	S'_2	$\Gamma_7 = [2]\#[1^2]\#[1^2]\#[2] \otimes [2]'$	1
		$\Gamma_8 = [2]\#[1^2]\#[1^2]\#[2] \otimes [1^2]'$	1
$[2]\#[1^2]\#[1^2]\#[1^2]$	E'	$\Gamma_9 = [2]\#[1^2]\#[1^2]\#[1^2] \otimes [1]' \uparrow S_2[S_2, S_2]$	2
$[1^2]\#[2]\#[2]\#[1^2]$	S'_2	$\Gamma_{10} = [1^2]\#[2]\#[2]\#[1^2] \otimes [2]'$	1
		$\Gamma_{11} = [1^2]\#[2]\#[2]\#[1^2] \otimes [1^2]'$	1
$[1^2]\#[2]\#[1^2]\#[1^2]$	E'	$\Gamma_{12} = [1^2]\#[2]\#[1^2]\#[1^2] \otimes [1]' \uparrow S_2[S_2, S_2]$	2
$[1^2]\#[1^2]\#[1^2]\#[1^2]$	S'_2	$\Gamma_{13} = [1^2]\#[1^2]\#[1^2]\#[1^2] \otimes [2]'$	1
		$\Gamma_{14} = [1^2]\#[1^2]\#[1^2]\#[1^2] \otimes [1^2]'$	1

Table 2. Conjugacy classes of $S_2[S_2, S_2]$, the generalized wreath product group of tetraphenyl and their orders

Class	Order	Class	Order
$\begin{bmatrix}20\\00\end{bmatrix}\begin{bmatrix}20\\00\end{bmatrix}$	1	$\begin{bmatrix}20\\00\end{bmatrix}\begin{bmatrix}00\\20\end{bmatrix}$	1
$\begin{bmatrix}10\\10\end{bmatrix}\begin{bmatrix}20\\00\end{bmatrix}$	2	$\begin{bmatrix}10\\10\end{bmatrix}\begin{bmatrix}00\\20\end{bmatrix}$	2
$\begin{bmatrix}00\\20\end{bmatrix}\begin{bmatrix}20\\00\end{bmatrix}$	1	$\begin{bmatrix}00\\20\end{bmatrix}\begin{bmatrix}00\\20\end{bmatrix}$	1
$\begin{bmatrix}20\\00\end{bmatrix}\begin{bmatrix}10\\10\end{bmatrix}$	2	$\begin{bmatrix}01\\00\end{bmatrix}\begin{bmatrix}01\\00\end{bmatrix}$	4
$\begin{bmatrix}00\\20\end{bmatrix}\begin{bmatrix}10\\10\end{bmatrix}$	2	$\begin{bmatrix}00\\01\end{bmatrix}\begin{bmatrix}01\\00\end{bmatrix}$	4
$\begin{bmatrix}10\\00\end{bmatrix}\begin{bmatrix}00\\10\end{bmatrix}\begin{bmatrix}10\\00\end{bmatrix}\begin{bmatrix}00\\10\end{bmatrix}$	2	$\begin{bmatrix}01\\00\end{bmatrix}\begin{bmatrix}00\\01\end{bmatrix}$	4
$\begin{bmatrix}10\\00\end{bmatrix}\begin{bmatrix}10\\00\end{bmatrix}\begin{bmatrix}00\\10\end{bmatrix}\begin{bmatrix}00\\10\end{bmatrix}$	2	$\begin{bmatrix}00\\01\end{bmatrix}\begin{bmatrix}00\\01\end{bmatrix}$	4

Table 3. The character table of the generalized wreath product $S_2[S_2, S_2]$, the permutation group of the non-rigid tetraphenyl in Fig. 2

Conj.	$\begin{bmatrix}20\\00\end{bmatrix}$	$\begin{bmatrix}10\\10\end{bmatrix}$	$\begin{bmatrix}00\\20\end{bmatrix}$	$\begin{bmatrix}20\\00\end{bmatrix}$	$\begin{bmatrix}00\\20\end{bmatrix}$	$\begin{bmatrix}10\\00\end{bmatrix}\begin{bmatrix}00\\10\end{bmatrix}$	$\begin{bmatrix}10\\00\end{bmatrix}\begin{bmatrix}10\\00\end{bmatrix}$	$\begin{bmatrix}20\\00\end{bmatrix}$	$\begin{bmatrix}10\\10\end{bmatrix}$	$\begin{bmatrix}00\\20\end{bmatrix}$	$\begin{bmatrix}01\\00\end{bmatrix}$	$\begin{bmatrix}00\\01\end{bmatrix}$	$\begin{bmatrix}01\\00\end{bmatrix}$	$\begin{bmatrix}00\\01\end{bmatrix}$
Class	$\begin{bmatrix}20\\00\end{bmatrix}$	$\begin{bmatrix}20\\00\end{bmatrix}$	$\begin{bmatrix}20\\00\end{bmatrix}$	$\begin{bmatrix}10\\10\end{bmatrix}$	$\begin{bmatrix}10\\10\end{bmatrix}$	$\begin{bmatrix}10\\00\end{bmatrix}\begin{bmatrix}00\\10\end{bmatrix}$	$\begin{bmatrix}00\\10\end{bmatrix}\begin{bmatrix}00\\10\end{bmatrix}$	$\begin{bmatrix}00\\20\end{bmatrix}$	$\begin{bmatrix}00\\20\end{bmatrix}$	$\begin{bmatrix}00\\20\end{bmatrix}$	$\begin{bmatrix}01\\00\end{bmatrix}$	$\begin{bmatrix}01\\00\end{bmatrix}$	$\begin{bmatrix}00\\01\end{bmatrix}$	$\begin{bmatrix}00\\01\end{bmatrix}$
Order	1	2	1	2	2	2	2	1	2	1	4	4	4	4
Γ_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
Γ_3	2	0	−2	2	−2	0	0	2	0	−2	0	0	0	0
Γ_4	2	2	2	0	0	0	0	−2	−2	−2	0	0	0	0
Γ_5	2	0	−2	0	0	−2	2	−2	0	2	0	0	0	0
Γ_6	2	0	−2	0	0	2	−2	−2	0	2	0	0	0	0
Γ_7	1	1	1	−1	−1	−1	−1	1	1	1	1	1	−1	−1
Γ_8	1	1	1	−1	−1	−1	−1	1	1	1	−1	−1	1	1
Γ_9	2	0	−2	−2	2	0	0	2	0	−2	0	0	0	0
Γ_{10}	1	−1	1	1	1	−1	−1	1	−1	1	1	−1	1	−1
Γ_{11}	1	−1	1	1	1	−1	−1	1	−1	1	−1	1	−1	1
Γ_{12}	2	−2	2	0	0	0	0	−2	2	−2	0	0	0	0
Γ_{13}	1	−1	1	−1	−1	1	1	1	−1	1	1	−1	−1	1
Γ_{14}	1	−1	1	−1	−1	1	1	1	−1	1	−1	1	1	−1

Because the inertia group is the identity group, distinction of rings within each Y set is necessary. This is done using the superfixes.

$$T(M)_{11}^{(1)} = \frac{1}{2}\left\{\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} \oplus \begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}\right\}, \tag{35}$$

$$T(M)_{11}^{(2)} = \frac{1}{2}\left\{\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} \ominus \begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}\right\}, \tag{36}$$

$$T(M)_{21}^{(1)} = \frac{1}{2}\left\{\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} \oplus \begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}\right\}, \tag{37}$$

$$T(M)_{21}^{(2)} = \frac{1}{2}\left\{\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} \oplus \begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}\right\}. \tag{38}$$

Hence,

$$\begin{aligned} P^{\Gamma_4} &= \frac{1}{8}\left[\left\{\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} \oplus \begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}\right\}\left\{\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} \ominus \begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}\right\}\right.\\ &\quad \times \left.\left\{\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} \oplus \begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}\right\}\left\{\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} \oplus \begin{bmatrix}0 & 0\\1 & 0\end{bmatrix}\right\}\right]\\ &= \frac{1}{36}\left\{2\begin{bmatrix}2 & 0\\0 & 0\end{bmatrix}\begin{bmatrix}2 & 0\\0 & 0\end{bmatrix} \oplus 4\begin{bmatrix}1 & 0\\1 & 0\end{bmatrix}\begin{bmatrix}2 & 0\\0 & 0\end{bmatrix}\right.\\ &\quad \oplus 2\begin{bmatrix}0 & 0\\2 & 0\end{bmatrix}\begin{bmatrix}2 & 0\\0 & 0\end{bmatrix} \ominus 2\begin{bmatrix}2 & 0\\0 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\2 & 0\end{bmatrix}\\ &\quad \left.\ominus 4\begin{bmatrix}1 & 0\\1 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\2 & 0\end{bmatrix} \ominus 2\begin{bmatrix}0 & 0\\2 & 0\end{bmatrix}\begin{bmatrix}0 & 0\\2 & 0\end{bmatrix}\right\}. \end{aligned} \tag{39}$$

Thus the coefficients 2, 4, 2 -2, -4, -2 are simply the products of the number of elements in the corresponding conjugacy classes and the character associated with an element in the respective classes (see Table 3).

5. Conclusion

In this paper we have developed a powerful cycle type matrix algebra to generate the characters of generalized wreath product groups. It has been shown that the character table of the generalized wreath product $G[H_1, H_2, \ldots, H_n]$ can be obtained using the generalized character cycle indices of G, and the cycle type matrices of $H_1, H_2, \ldots, H_n$, through powerful cycle type matrix substitutions in the GCCI of the group G. A non-rigid tetraphenyl molecule has been used as an example to illustrate our method. The character table of the non-rigid tetraphenyl has been obtained for the first time.

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