Symmetry Groups of Chemical Graphs

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Abstract

The symmetry groups of all trees are shown to be expressible as generalized wreath products by a tree pruning algorithm. The symmetry groups of certain cyclic graphs which can be expresssed as generalized compositions are also shown to be generalized wreath products. The symmetry groups of complete multipartite graphs can be obtained in a similar manner. Character tables of symmetry groups of certain chemical graphs are also obtained.

1. Introduction

Graphs are potentially useful in representing interactions (quantum mechanical or statistical mechanical), isomer interconversions, interrelationships in some observations related to molecular structure, chemical reaction networks, etc. A selection of review topics of such applications appears in the recent book of Balaban [1]. Graphs provide diagrammatic representations of many abstract quantities involved in physics or chemistry. Feynman diagrams of manybody interactions [2] and Mayer-Mayer graphs [1] are classical examples of such graphs in chemical physics. Consequently, it is important to study the symmetry properties of these graphs, which in turn reflect the symmetry properties of the associated interactions or phenomena they represent.

Symmetry elements of a graph do not depend on its pictorial stereorepresentation but rather on how the various vertices are connected. The same graph can be drawn in different stereorepresentations [3] which apparently may look to have different symmetry elements, yet their symmetry groups can be identical. It is this aspect which makes the symmetry group of a graph and hence its recognition, different from the conventional molecular point groups and space groups. Randić [4–8] took some pioneering steps in the study of the symmetry properties and recognition of graphs of chemical interest. In these series of papers Randić outlined methods for searching symmetries in graphs. In this paper we develop techniques for obtaining the symmetry groups of graphs as permutation groups of their vertices. Algorithms developed here are based on expressing bigger graphs as products of smaller graphs iteratively and expressing the symmetry groups of bigger graphs as group products (generalized wreath products) of smaller graphs. The need for such algorithms is evident since we

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need to obtain further information concerning the symmetry groups of these graphs such as their character tables etc., as they are needed in many chemical and physical applications like selection rules, symmetry correlations, spectra, etc. For example, it was shown by the present author [9] that NMR interactions can be represented by graphs and their automorphism groups which preserve NMR couplings are NMR groups. Further, as we will show in future investigations character tables of the symmetry groups of chemical graphs have important applications in predicting the symmetry of spectra of graphs and thus the NMR spectra. For these reasons we undertake this investigation.

In Section 2 a pruning algorithm for trees is developed by which the symmetry groups of all trees can be expressed as generalized wreath products iteratively. Section 3 discusses the symmetry groups of cyclic graphs particularly those which can be expressed as generalized compositions and in the last section the symmetry groups of multipartite graphs is considered.

2. Pruning Algorithm for Trees

A tree is a connected graph that has no cycles. In this section we show that the symmetry groups of trees can be obtained by pruning the tree successively until we obtain an unbranched tree. We start with the definition of the symmetry group of a graph.

The symmetry group of a graph Γ or its automorphism group consists of permutations of the vertices of Γ that preserve the adjacency matrix of a graph defined by:

$$A_{ij} = \begin{cases} 1, \text{ if } i \text{ and } j \text{ are connected} \\ 0, \text{ otherwise} \end{cases}.$$

Equivalently, the symmetry group of Γ consists of permutations whose permutation matrices P satisfy

$$PAP^{-1} = A. \tag{1}$$

The vertices of degree 1 which are attached to the same vertex can be permuted among themselves and this would leave the adjacency matrix invariant. This motivates the formulation of a pruning algorithm by which we can successively break down the tree into an unbranched tree. For example, let us consider the tree shown in Figure 1. This tree has 4 sets of vertices each set containing 2
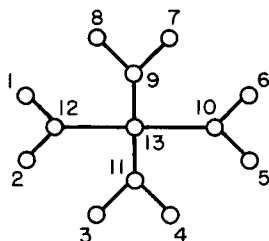

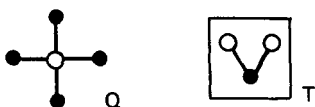
Figure 1. A "tree" with 13 vertices.

Figure 2. A "tree" and the type resulting from the application of pruning algorithm to the tree shown in Figure 1.

vertices that can be permuted. All the four sets are symmetrically equivalent and hence they can be permuted among themselves. This is the philosophy behind the pruning procedure. First, the set of vertices of degree 1 that are attached to the same vertex is identified. Then the tree is pruned at these joints. This pruning process gives rise to a graph product formulated by the author [10] known as root-to-root product. The joints of a tree which are the vertices of degree more than 1 are distinguishable from the other vertices and hence are considered as roots. For the tree shown in Figure 1 the vertices 9, 10, 11, 12 and 13 are the roots. The four sets of vertices of degree are {1, 2}, {3, 4}, {5, 6}, and {7, 8}. Any permutation within a set leaves the adjacency matrix invariant and any permutation of the sets also leaves the adjacency matrix invariant. Let us group all vertices of same degree in the same set. For example, for the tree shown in Figure 1 three such sets are $Y_1 = \{1, 2, 3, 4, 5, 6, 7, 8\}$, $Y_2 = \{9, 10, 11, 12\}$, and $Y_3 = \{13\}$. Then the tree in Figure 1 can be broken down to trees shown in Figure 2. Equivalently, the tree in Figure 1 is obtainable by attaching each black dot in Q and a black dot of a copy of the type T. Thus Qs and Ts are generated by pruning the tree at joints. Now we are left with a tree which is smaller than the original tree. However, in this example Q is still branched and hence we have to prune it again. The result of pruning Q is shown in Figure 3. Now we have an unbranched tree (in this case a tree containing just one vertex). The symmetry group of an unbranched tree is either E or S_2, where E is the group containing just the identity operation and S_2 contains 2 permutations. The former is the symmetry group of a nonsymmetric unbranched tree while the latter is the symmetry group of a symmetric unbranched tree. At every stage of pruning the symmetry group of the unpruned tree is a generalized wreath product of the symmetry group of the pruned tree and the symmetry groups of the types generated in the process of pruning. For example, the symmetry group of the unpruned tree in Figure 2 is $E[S_4]$ which is isomorphic to S_4. The symmetry group of the tree shown in Figure 1 is thus $S_4[S_2]$ by this algorithm. The order of this group is 384. The character table of this group can be obtained using the representation theory of generalized wreath products developed by the author

Figure 3. A "tree" and the type resulting from the application of pruning algorithm to the tree shown in Figure 2.

[11] and the elegant generating function techniques for characters [12–13]. The character table is shown in Table I. The conjugacy classes can be obtained by the method discussed in Ref. 11. This table is in agreement with the compound character table $[8]+[62]+[4^2]+[42^2]+[2^4]$ found in Littlewood [14].

TABLE I.   Character table of the symmetry group of the graph shown in Figure 1.

	1	(12)	(12)(34)	(12)(34)(56)	(12)(34)(56)(78)	(12)(28)(9,12)	(17)(28)(56)(9,12)	(17)(28)(34)(56)(9,12)	(1827)(9,12)	(1827)(56)(9,12)	(1827)(34)(56)(9,12)	(175)(286)(9,10,12)	(175)(286)(34)(9,10,12)	(17528 6)(9,10,12)	(17528 6)(34)(9,10,12)	(17)(28)(35)(46)(9,12)(10,11)	(1827)(35)(46)(9,12)(10,11)	(1827)(3645)(9,12)(10,11)	(1753)(2864)(12,9,10,11)	(18642753)(12,9,10,11)
	1	4	6	4	1	12	24	12	12	24	12	32	32	32	32	12	24	12	48	48
A_1	1	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	1	-1
A_3	1	1	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	-1	1
E_1	2	2	2	2	2	0	0	0	0	0	0	-1	-1	-1	-1	2	2	2	0	0
E_2	2	-2	2	-2	2	0	0	0	0	0	0	-1	1	1	-1	2	-2	2	0	0
F_1	3	3	3	3	3	1	1	1	1	1	1	0	0	0	0	-1	-1	-1	-1	-1
F_2	3	-3	3	-3	3	1	-1	1	-1	1	-1	0	0	0	0	-1	1	-1	-1	1
F_3	3	3	3	3	3	-1	-1	-1	-1	-1	-1	0	0	0	0	-1	-1	-1	1	1
F_4	3	-3	3	-3	3	-1	1	-1	1	-1	1	0	0	0	0	-1	1	-1	-1	-1
G_1	4	2	0	-2	-4	2	0	-2	2	0	-2	1	-1	1	-1	0	0	0	0	0
G_2	4	-2	0	2	-4	2	0	-2	-2	0	2	1	1	-1	-1	0	0	0	0	0
G_3	4	2	0	-2	-4	-2	0	2	-2	0	2	1	-1	1	-1	0	0	0	0	0
G_4	4	-2	0	2	-4	-2	0	2	2	0	-2	1	1	-1	-1	0	0	0	0	0
I_1	6	0	-2	0	6	2	0	2	0	-2	0	0	0	0	0	2	0	-2	0	0
I_2	6	0	-2	0	6	-2	0	-2	0	2	0	0	0	0	0	2	0	-2	0	0
I_3	6	0	-2	0	6	0	-2	0	2	0	-2	0	0	0	0	0	2	0	2	0
I_4	6	0	-2	0	6	0	2	0	-2	0	2	0	0	0	0	0	-2	0	2	0
K_1	8	4	0	-4	-8	0	0	0	0	0	0	-1	1	-1	1	0	0	0	0	0
K_2	8	-4	0	4	-8	0	0	0	0	0	0	-1	-1	1	1	0	0	0	0	0

3. The Symmetry Groups of Generalized Compositions

The composition of two graphs Γ_1 and Γ_2 denoted as $\Gamma_1[\Gamma_2]$ is obtained by replacing each vertex of Γ_1 by a copy of Γ_2 and each line of Γ_1 by the lines which join the corresponding copies of Γ_2. Harary [15] showed that the symmetry group of $\Gamma_1[\Gamma_2]$ is the wreath product $G[H]$ if G is the symmetry group of Γ_1 and H is the symmetry group of Γ_2 provided not both Γ_1 and Γ_2 are complete. If both Γ_1 and Γ_2 are complete then the symmetry group is S_{nm} if n and m are the number of vertices in Γ_1 and Γ_2, respectively. This result can be generalized to generalized composition of graphs defined below.

A generalized composition of a graph Q with various "types" $T_1, T_2, \ldots$ denoted as $Q[T_1, T_2, \ldots]$ is obtained as follows. Let the vertices of Q be

partitioned into sets Y_1, $Y_2, \ldots, Y_t$. Then the generalized composition $Q[T_1, T_2, \ldots, T_t]$ is obtained by replacing each vertex of Q in Y_i by a copy of the type T_i. For example, a graph Q, types T_1, T_2, and the generalized composition $Q[T_1, T_2]$ are shown in Figure 4. The vertices of Q are partitioned into the Y sets $Y_1 = \{1, 3\}$ and $Y_2 = \{2\}$.
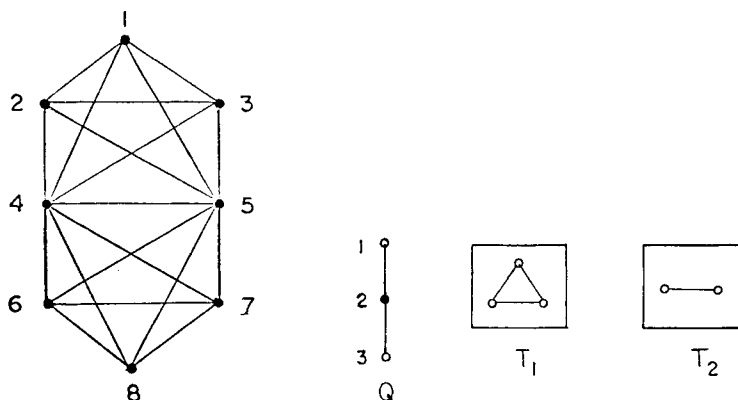

Figure 4. A graph expressed as generalized composition.

The symmetry group of generalized composition can be obtained by extending Harary's method [15] for obtaining the symmetry group of composition of two graphs. However, this is not a straightforward extension since generalized compositions cause problems when the induced subgraph of any Y_i and the corresponding type T_i are both complete. When such a possibility does not exist in the graph, the symmetry group of $Q[T_1, T_2, \ldots, T_t]$ is the generalized wreath product $G[H_1, H_2, \ldots, H_t]$, where G is the symmetry group of Q and H_i is the symmetry group of T_i ($i = 1, 2, \ldots, t$). This is because each isomorphism of $Q[T_1, T_2, \ldots, T_t]$ that preserves its adjacency matrix can be obtained by permuting the copies of $T_1, T_2, \ldots, T_t$ with an element of the symmetry group of Q. Then the isomorphism between $y_{ij} \in Y_i$, and T_i can be induced on separate representatives which preserves the adjacency matrix. Since this is the way generalized wreath product $G[H_1, H_2, \ldots, H_t]$ is constructed, we have the result. When the induced subgraph of Y_i and T_i are complete, the component induced by the vertices $(Y_i, V(T_i))$ of $Q[T_1, T_2, \ldots, T_t]$ is complete and hence the symmetry group of the induced subgraph of $(Y_i, V(T_i))$ is $S_{|Y_i||V(T_i)|}$, where $V(T_i)$ is the set of vertices of T_i. If the graph $Q - G(Y_i)$ where $G(Y_i)$ is the induced subgraph of Y_i does not contain any other complete subgraph induced by Y_j and a complete T_j then the symmetry group of $Q[T_1, T_2, \ldots, T_t]$ is $S_{|Y_i||V(T_i)|} \times G_{Q-G(Y_i)}[H_1, H_2, \ldots, \hat{H}_i, \ldots, H_t]$, where a hat on a variable denotes the omission of that variable and $G_{Q-G(Y_i)}$ is the symmetry on group of the graph $Q - G(Y_i)$. If the graph $G - G(Y_i)$ contains a complete subgraph induced by Y_j and if T_j is complete, then this process is repeated until we reach a graph that does not contain such a pair. Then the

symmetry group of $Q[T_1, T_2, \ldots, T_t]$ is

$$\underset{i=1}{\overset{k}{\times}} S_{|Y_i||V(T_i)|} \times G_{Q-Q'}[H_{k+1}, \ldots, H_t]$$

where

$$Q' = \sum_{i=1}^{k} G(Y_i),$$

and $G_{Q-Q'}$ is the symmetry group of the graph $Q - Q'$. We assumed that the pairs of complete subgraphs induced by Y_i and T_i are $i = 1, 2, \ldots, k$. Note that this result specializes to the result that we obtained when there is no complete subgraph induced by any Y_i and a complete T_i, since Q' is a null graph in this case.

Let us illustrate the symmetry groups of generalized compositions with two examples which exemplify these two cases. As an example of the first case let us consider the graph shown in Figure 4. Since none of the subgraphs induced by Y_1 or Y_2 is complete this belongs to the first case. The symmetry groups of Q, T_1, and T_2 are S_2, S_3, and S_2 respectively. Thus the symmetry group of the graph is $S_2[S_3, S_2]$. Character table of this group was already obtained by the author (Ref. 11, see Table IV).

Consider the graph shown in Figure 5 as an example of the second case. The Y sets are $Y_1 = \{1, 2, 3\}$, $Y_2 = \{6, 7, 8, 9\}$, $Y_3 = \{4, 5\}$. Since the induced subgraphs
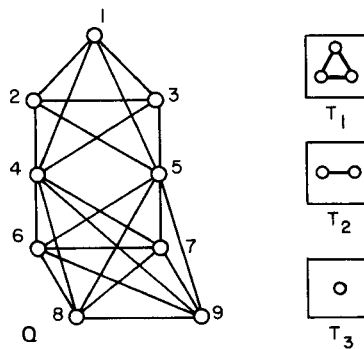

Figure 5. A graph expressed as generalized composition which contains two pairs of subgraphs induced by the sets Y_1 and Y_2 (which are complete) and the complete types T_1 and T_2.

of Y_1, Y_2 are complete and T_1 and T_2 are complete, we need to consider the graph $Q - G(Y_1) - G(Y_2)$ which is the subgraph induced by Y_3. This graph contains just two disconnected vertices. Thus the symmetry group of this component is S_2. Therefore, the symmetry group of the whole graph $Q[T_1, T_2, T_3]$, is

$$S_{|Y_1||V(T_1)|} \times S_{|Y_2||V(T_2)|} \times S_2[S_2]$$

This is equal to $S_9 \times S_8 \times S_2[S_2]$. The order of this group is $9!\,8!\,8$. The character table of this group is the Kronecker product of the character tables of S_9, S_8 and $S_2[S_2]$ which can be found.

4. The Symmetry Groups of Complete Multipartite Graphs

Let $X_1, X_2, \ldots, X_n$ be n vertex sets and let $|X_i| = t_i$ ($i = 1, n$). Then a complete n-partite graph with the vertex set $U_{i=1}^n X_i$ is a graph which has no edges between any two vertices in any set X_i and all vertices in X_i and X_j ($i \neq j$) are connected for $i = 1$, $n - 1$, and $j = i + 1$, n. The symmetry group of such a graph can be found using the methodology of Section 3. A n-partite graph can be expressed as a generalized composition by condensing the vertices of X_i into a single vertex and generating the corresponding representative of T_i. All vertices that have the same representative are grouped in the same set Y_i and the corresponding representative is a copy of the same type T_i. Types T_i are thus disconnected. Let the symmetry group of the quotient graph Q be G. $S_{|V(T_i)|}$ is the symmetry group of the type T_i. Thus the symmetry group of the complete n-partite graph is

$$G[S_{|V(T_1)|}, S_{|V(T_2)|}, \ldots]$$

To illustrate consider the three-partite graph which has been expressed as a generalized composition in Figure 6. The Y sets are $Y_1 = \{1, 2\}$ and $Y_2 = \{3\}$.
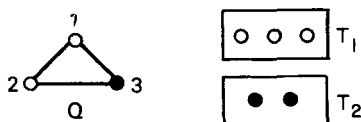

Figure 6. A 3-partite graph expressed as generalized composition.

The symmetry groups of the types T_1 and T_2 are S_3 and S_2, respectively. Thus the symmetry group of the graph shown in Figure 6 is $S_2[S_3, S_2]$. This group is isomorphic to the symmetry group of graph in Figure 4 whose character table was obtained in Ref. 11.

Acknowledgements

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