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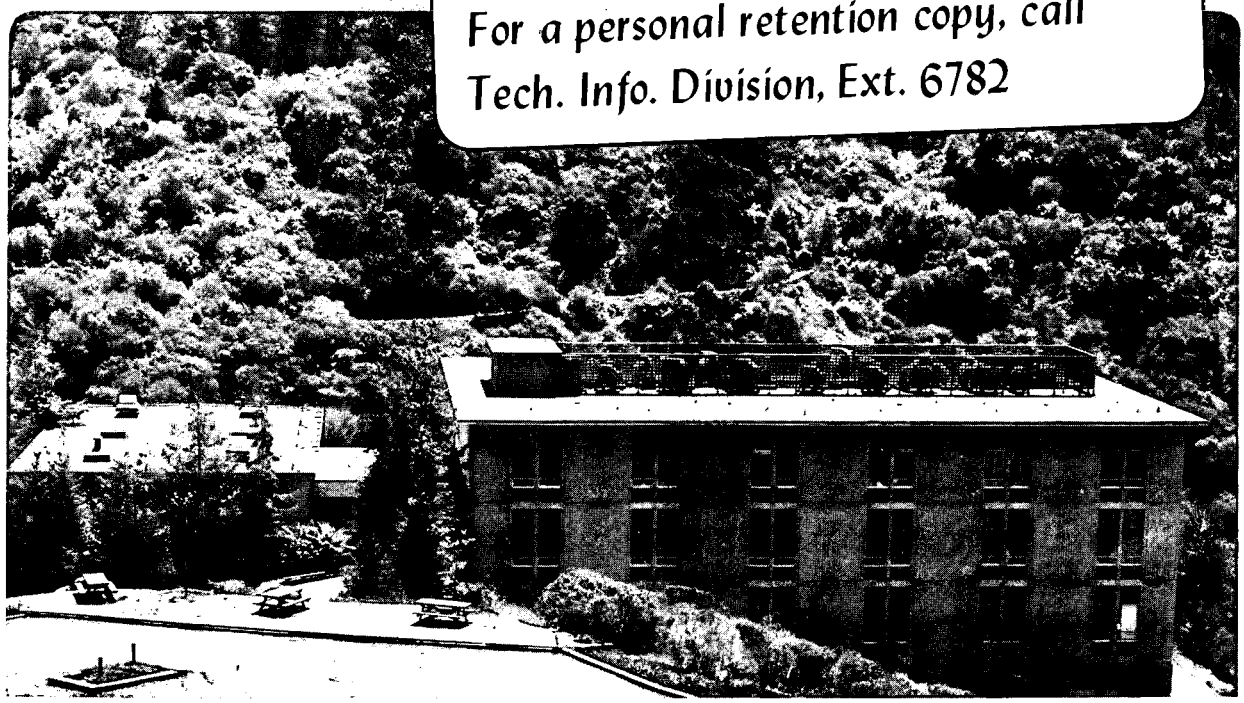

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A Method for Constructing Isomerization Reactions

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Abstract

A method is formulated for enumerating and constructing isomerization reactions of molecules exhibiting large amplitude non-rigid motions. This method not only enumerates the isomers of non-rigid molecules and the corresponding rigid molecules but also the symmetry species spanned by the equivalent structures whose representative is an isomer. Consequently, using the method of correlating the symmetry species of a group to the symmetry species of its subgroup the splitting patterns of isomers of non-rigid molecule to those of rigid molecule are obtained. This provides an elegant method for both enumerating and constructing reaction graphs. The method is illustrated with examples.

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1. Introduction

In recent years several papers[1-7] have appeared that concern representations and enumerations of dynamic processes in molecules exhibiting large amplitude motions. The inter-relationship among a set of rigid isomers that are transformable into one another by non-rigid symmetry operations can be described by the associated diagram called a reaction graph. A reaction graph as formulated in reference 7b is a diagram with vertices and edges, vertices representing isomers of the rigid molecules and the edges representing interconversions of such rigid isomers by operations in the rotation group of the non-rigid molecule. There are several other topological schemes and representations of processes of interest in dynamic stereochemistry. An excellent review of such schemes can be found in the papers of Mislow[1] or the recent book by Balaban.[4] Several such chemical applications of graph theory can be found in the papers of Randić.[3] It is known that the isomers of molecules can be characterized and enumerated very elegantly harnessing the symmetry of the unsubstituted molecule.[10-13] The combinatorial structures constructed using the symmetry of the molecule are generators and enumerators of such phenomena. One combinatorial structure is the well-known cycle index of a group,[4,12-16] which is the generator of isomers.

The cycle indices have been employed in chemical applications by several authors.[1,3-11] In this paper we introduce and use a more general and powerful generator called a generalized character cycle index (hereafter abbreviated as GCCI). A GCCI is a cycle index that also has the character of the irreducible representation to which it corresponds. Consequently, GCCI's are generators of not only isomers (patterns in

Pólya terminology[12]) but also the irreducible representations spanned by the set of functions in each pattern or the equivalence class. Generation of symmetry species spanned by the set of equivalent molecular structures corresponding to an isomer is important. This is because to enumerate and construct isomerization reactions all that one needs to do is the correlation of the irreducible representations of the molecular rotation group of the non-rigid molecule to those of the molecular rotation group of the rigid molecule. The latter is a subgroup of the former so that in general, an irreducible representation of the former is a reducible representation of the latter. Such correlation of the symmetry species of group to subgroup is quite common in spectroscopy and other problems in chemical physics.[17] In this paper we employ this technique to correlate the isomers of non-rigid molecule to the rigid molecule by way of correlating the symmetry species contained in the set of structures that represent an isomer. In general, an isomer of a non-rigid molecule "splits" into more isomers when correlated to rigid molecular symmetry.

Section II discusses the theory and in the last section we outline the method of correlation and enumeration of isomerization reactions.

2. Theory

Let G be the rotational subgroup of the molecular symmetry group. We use the rotation subgroup rather than the complete symmetry group since by definition, isomers are structures that are not transformable into one another by rotations. Let D be the set of unsubstituted sites and let R be the set of substituents. Then a molecular structure can be formed by a map from D to R. To illustrate, if one denotes the 5 unsubstituted sites of a trigonal bipyramid by D = {1,2,3,4,5} and R as the

set {Cℓ, Br} then a structure corresponding to the molecule $PCℓ_3Br_2$ is generated by the following map f_1 from D to R.

$$f_1(1) = Cℓ$$

$$f_1(2) = Cℓ$$

$$f_1(3) = Cℓ$$

$$f_1(4) = Br$$

$$f_1(5) = Br.$$

A permutation g in G permutes the elements in D; in turn g also permutes the maps from D to R. Thus two molecular structures or maps from D to R are equivalent if they are transformable into one another. Formally, two structures f_1 and f_2 are equivalent if there is a $g \varepsilon G$ such that

$$f_1(d) = f_2(gd), \text{ for every } d \varepsilon D.$$

For example, the map f_2 shown below is equivalent to f_1 in the non-rigid rotation group of this molecule which is S_5 (S_n stands for the set of n! permutations).

$$f_2(1) = Br$$

$$f_2(2) = Br$$

$$f_2(3) = Cℓ$$

$$f_2(4) = Cℓ$$

$$f_2(5) = Cℓ.$$

This is because f_1 and f_2 are transformable by the above recipe, for example, if g = (14)(25). All equivalent maps can be grouped together

in a set and any structure in that set is an isomer. The set of equivalent structures corresponding to any isomer transform into each other under the operations of G and consequently, in general span a reducible representation of G which can be decomposed into irreducible components.

Let us define the generalized character cycle index (GCCI) of a group G corresponding to character χ of an irreducible representation Γ of G as

$$P_G^{\chi} = \frac{1}{|G|} \sum_{g \in G} \chi(g)\, x_1^{b_1} x_2^{b_2} \ldots\ldots x_n^{b_n}$$

where $x_1^{b_1} x_2^{b_2} \ldots x_n^{b_n}$ is a representation of a typical permutation g in G having b_1 cycles of length 1, b_2 cycles of length 2,....,b_n cycles of length n. To illustrate, permutations (12) (345) and (1) (23) (45) would have the representations x_2x_3 and $x_1x_2^2$, respectively. In order to book-keep the number of various substituents occurring in a structure let us introduce the concept of weight of a structure and substituent. With each substituent $r \in R$, let us associate a formal symbol w(r). Then the weight of any structure f is defined by the product of the weights of the corresponding images. In symbols,

$$W(f) = \prod_{d \in D} w(f(d)).$$

To illustrate, if the weight associated with Cℓ is w_1 and Br is w_2 then the weight of the structure $PCℓ_3Br_2$ is $w_1^3w_2^2$. Isomers are structures that have the same weight and yet not transformale into one another by rotation.

In this set up Williamson[15] and more recently Merris[16] (who generalized Williamson's formulation) showed that the generator of the irreducible representations contained in the set of all structures is given by the following Pólya-like substitution in the GCCI.

$$G.F.^{\chi} = P_G^{\chi}[x_k \rightarrow \sum_{r\epsilon R} (w(r))^k].$$

The coefficient of a typical term $w_1^{b_1} w_2^{b_2}....$ in G.F. gives the number of times χ occurs in the set of structures with the weight $w_1^{b_1} w_2^{b_2}....$.

Let us illustrate the above method with an example. The character table of the rotational subgroup of the non-rigid trigonal bipyramid molecule is shown in Table 1. Table 2 contains all the GCCI's of this molecule. Consider the H_1 representation of this molecule. We consider the case of 3 different substituents with the weights a, b and c. The GCCI and the G.F.^{H_1} are shown below.

$$GCCI^{H_1} = \frac{1}{120}[5x_1^5 + 10\, x_1^3x_2 - 20\, x_1^2x_3 - 30\, x_1x_4 + 15\, x_1x_2^2 + 20\, x_2x_3]$$

$$G.F.^{H_1} = GCCI^{H_1}(x_k \rightarrow a^k + b^k + c^k)$$

$$= \frac{1}{120}[5(a+b+c)^5 + 10(a+b+c)^3\,(a^2+b^2+c^2) - 20(a+b+c)^2$$

$$(a^3+b^3+c^3) - 30(a+b+c)(a^4+b^4+c^4) + 15(a+b+c)\,(a^2+b^2+c^2)^2$$

$$+ 20(a^2+b^2+c^2)\,(a^3+b^3+c^3)]$$

$$= a^3b^2 + a^2b^3 + a^3bc + 2a^2b^2c + ab^3c + a^3c^2 + 2a^2bc^2$$

$$+ 2ab^2c^2 + b^3c^2 + a^2c^3 + abc^3 + b^2c^3.$$

Thus there is one H_1 representation in the set of structures with the formula $PC\ell_3Br_2$, 2 H_1 representations in the set of structures with the formula $PC\ell_2Br_2$ I, etc. The GCCI corresponding to the totally symmetric representation enumerates the isomers since this GCCI is just the ordinary cycle index used by several authors for enumerating isomers.[1,4-10] We will use the formalism outlined here in the next section to enumerate isomerization reactions.

3. Enumeration of Isomerization Reactions

We start with the trigonal bipyramidal compounds which exhibit large amplitude non-rigid motions by way of the pseudorotation proposed by Berry, now well-known as Berry mechanism. The rotational subgroup of this non-rigid molecule is the group S_5, whose character table and GCCI's have already been obtained. Table 3 shows the generating functions for 3 substituents with the weights a, b and c. The first row in this table shows the various terms appearing in the generating function. All the subsequent rows give the coefficients of the corresponding terms for the irreducible representations they stand for. We consider a particular molecule with the formula Px_2y_2z as an example. The enumerators corresponding to this formula are the coefficients of a^2b^2c in the various generating functions. The coefficient of a^2b^2c in the totally symmetric representation A_1 gives the number of isomers which is just 1 in this case. There are $\binom{5}{2\ 2\ 1} = 30$ structures (maps) that are equivalent and they all represent one isomer. These 30 structures span the representation $A_1 + 2G_1 + 2H_1 + H_2 + I$. This is obtained immediately by collecting the coefficient of a^2b^2c in the generating function of each irreducible representation. For example, the coefficient of a^2b^2c in G_1 is 2; in H_1 it is 2, in H_2 it is 1 and in I it is 1. Thus we arrive at the above result. Isomerization reactions are obtained when one finds the set of representations spanned by the same 30. Structures in the rotational subgroup of the rigid molecule which is D_3. This is easily done by correlating the species A_1, G_1, H_1, H_2 and I to the species of the group D_3. The character table of D_3 and the correlation table of the symmetry species of S_5 to D_3 are shown in tables 4 and 5, respectively. Consequently, these 30 structures span the representation $6A_1 + 4A_2 + 10E$. Note that these sets of

maps contain $6A_1$ representations in D_3 when they contained only one A_1 in S_5. Since the number of A_1 representations gives the number of isomers we arrive at the conclusion that the single isomer of the non-rigid molecule Px_2y_2z splits into 6 isomers when the molecule becomes rigid. Conversely, the 6 isomers of the rigid molecule are transformed into one another by pseudo-rotation. This is represented by the reaction graph in Figure 1. We recall from Ref. 7b that a reaction graph has an edge between two vertices i and j if the rigid isomers i and j are transformable by a rotation in the non-rigid molecular group. Consequently, the reaction graph contains components that are always complete. Hence once we know the number of vertices in the reaction graph, the number of components and the number of vertices in each component, the reaction graph is immediately constructed.

Let us illustrate this procedure with another non-trivial example of a triphenyl which exhibits 2-fold rotation around the bond connecting phenyl rings. The character table of the molecular symmetry group of this molecule was obtained by the present author.[8] (c.f., Table V of Ref. 8). The rotational subgroup of the rigid molecule is easily seen to be D_2. The generating functions for the non-rigid molecule with 3 substituents can be obtained with the procedure in Section 2. Let us consider triphenyls with the formula $C_{18}H_{12}X_2$. There are 21 isomers (shown in Table 6 with the labels in Figure 2) for the non-rigid molecule since the coefficient of $a^{12}b^2$ is 21 in the generating function corresponding to the A_1 representation. In Table 7 we show the irreducible representations spanned by the set of equivalent structures whose representative is the isomer indicated in the first column. Table 8 is the correlation table of symmetry species of the non-rigid rotation group to those of the rigid rotation group. In Table 9 we have the correlation

of isomers obtained by way of correlating the symmetry species contained in the corresponding equivalent structures. From this table one can infer that isomers 9, 10, 11, 12, 16, 17 and 18 split; each of them split into 2 isomers when correlated to rigid structure. All the other isomers do not split. This is shown in the reaction graph in Figure 3.

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Table 1. The character table of S_5, the rotational subgroup of the non-rigid trigonal bipyramidal phosphorous compounds

Γ	E	(12)	(123)	(1234)	(12)(34)	(12)(345)	(12345)
Order	1	10	20	30	15	20	24
A_1	1	1	1	1	1	1	1
A_2	1	-1	1	-1	1	-1	1
G_1	4	2	1	0	0	-1	-1
G_2	4	-2	1	0	0	1	-1
H_1	5	1	-1	-1	1	1	0
H_2	5	-1	-1	1	1	-1	0
I	6	0	0	0	-2	0	1

Table 2. GCCI's of the group in Table 1. 120 P_G^{χ} are shown below

Γ	x_1^5	$x_1^3x_2$	$x_1^2x_3$	x_1x_4	$x_1x_2^2$	x_2x_3	x_5
A_1	1	10	20	30	15	20	24
A_2	1	-10	20	-30	15	-20	24
G_1	4	20	20	0	0	-20	-24
G_2	4	-20	20	0	0	20	-24
H_1	5	10	-20	-30	15	20	0
H_2	5	-10	-20	30	15	-20	0
I	6	0	0	0	-30	0	24

Table 3. Generating functions for non-rigid phosphrous compounds with at most 3 substituents

	a^5	a^4b	a^3b^2	a^2b^3	ab^4	b^5	a^4c	a^3bc	a^2b^2c	ab^3c	b^4c	a^3c^2	a^2bc^2	ab^2c^2	b^3c^2	a^2c^3	abc^3	b^2c^3	ac^4	bc^4	c^5
A_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
A_2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
G_1	0	1	1	1	1	0	1	2	2	2	1	1	2	2	1	1	2	1	1	1	0
G_2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H_1	0	0	1	1	0	0	0	1	2	1	0	1	2	2	1	1	1	1	0	0	0
H_2	0	0	0	0	0	0	0	0	1	0	0	0	1	1	0	0	0	0	0	0	0
I	0	0	0	0	0	0	0	1	1	1	0	0	1	1	0	0	1	0	0	0	0

Table 4. Character table of D_3

D_3	E	(123)	(12)(34)
Order	1	2	3
A_1	1	1	1
A_2	1	+1	-1
E	2	-1	0

Table 5. Correlation of symmetry species of S_5 to D_3

S_5	E	(123)	(12)(34)	D_3
A_1	1	1	1	A_1
A_2	1	1	1	A_1
G_1	4	1	0	$A_1 + A_2 + E$
G_2	4	1	0	$A_1 + A_2 + E$
H_1	5	-1	1	$A_1 + 2E$
H_2	5	-1	1	$A_1 + 2E$
I	6	0	-2	$2A_2 + 2E$

Table 6. The 21 isomers of the disubstituted non-rigid triphenyl. The positions of the substituent x's are indicated under the appropriate column. This table should be read in conjunction with Figure 2

Isomer	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1				x	x									
2	x	x												
3		x		x										
4	x			x										
5	x				x									
6	x		x											
7		x				x								
8		x					x							
9	x					x								
10	x						x							
11				x		x								
12				x			x							
13		x												x
14		x									x			
15		x										x		
16	x													x
17	x										x			
18				x										x
19						x	x							
20						x			x					
21						x		x						

Table 7. The irreducible representations spanned by the equivalent structures in each isomer

Isomer	No. of equivalent structures contained in this isomer	Irreducible representations
1	2	$A_1' + B_1'$
2	4	$A_1' + B_1' + E'$
3	4	$A_1' + B_1' + E'$
4	4	$A_1' + B_1' + E'$
5	4	$A_1' + B_1' + E'$
6	2	$A_1' + B_1'$
7	4	$A_1' + A_1'' + B_1' + B_1''$
8	4	$A_1' + A_1'' + B_1' + B_1''$
9	8	$A_1' + B_1' + E' + A_1'' + B_1'' + E''$
10	8	$A_1' + B_1' + E' + A_1'' + B_1'' + E''$
11	8	$A_1' + B_1' + E' + A_1'' + B_1'' + E''$
12	8	$A_1' + B_1' + E' + A_1'' + B_1'' + E''$
13	4	$A_1' + B_1' + E'$
14	4	$A_1' + B_1' + E'$
15	1	A_1'
16	8	$A_1' + B_1' + A_2' + B_2' + 2E'$
17	4	$A_1' + B_2' + E'$
18	4	$A_1' + B_2' + E'$
19	2	$A_1' + A_1''$
20	2	$A_1' + A_1''$
21	2	$A_1' + A_1''$

Table 8. Correlation of symmetry species of the non-rigid triphenyl to rigid triphenyl. The labels of the nuclei are as in Fig. 2

G_{16}	E	(1,3)(4,5)(6,9)(7,8)(10,14)(11,13)	(1,13)(2,12)(3,11)(4,10)(5,14)(6,7)(8,9)	(1,11)(2,12)(3,13)(4,14)(5,10)(6,8)(7,9)	D_2
A_1'	1	1	1	1	A
B_1'	1	1	-1	-1	B_1
A_2'	1	1	-1	-1	B_1
B_2'	1	1	1	1	A
A_1''	1	-1	-1	1	B_3
B_1''	1	-1	1	-1	B_2
A_2''	1	-1	1	-1	B_2
B_2''	1	-1	-1	1	B_3
E'	2	-2	0	0	$B_2 + B_3$
E''	2	+2	0	0	$A + B_1$

Table 9. Correlation of structures in each isomer of the triphenyl molecule. Number of rigid isomers corresponding to a non-rigid isomer is the number A representations

Non-rigid Isomer	Irreducible Representations G_{16}	D_2
1	$A_1' + B_1'$	$A + B_1$
2	$A_1' + B_1' + E'$	$A + B_1 + B_2 + B_3$
3	$A_1' + B_1' + E'$	$A + B_1 + B_2 + B_3$
4	$A_1' + B_1' + E'$	$A + B_1 + B_2 + B_3$
5	$A_1' + B_1' + E'$	$A + B_1 + B_2 + B_3$
6	$A_1' + B_1'$	$A + B_1$
7	$A_1' + A_1'' + B_1' + B_1''$	$A + B_1 + B_2 + B_3$
8	$A_1' + A_1'' + B_1' + B_1''$	$A + B_1 + B_2 + B_3$
9	$A_1' + B_1' + E' + A_1'' + B_1'' + E''$	$2A + 2B_1 + 2B_2 + 2B_3$
10	$A_1' + B_1' + E' + A_1'' + B_1'' + E''$	$2A + 2B_1 + 2B_2 + 2B_3$
11	$A_1' + B_1' + E' + A_1'' + B_1'' + E''$	$2A + 2B_1 + 2B_2 + 2B_3$
12	$A_1' + B_1' + E' + A_1'' + B_1'' + E''$	$2A + 2B_1 + 2B_2 + 2B_3$
13	$A_1' + B_1' + E'$	$A + B_1 + B_2 + B_3$
14	$A_1' + B_1' + E'$	$A + B_1 + B_2 + B_3$
15	A_1'	A
16	$A_1' + B_1' + A_2' + B_2' + 2E'$	$2A + 2B_1 + 2B_2 + 2B_3$
17	$A_1' + B_2' + E'$	$2A + B_2 + B_3$
18	$A_1' + B_2' + E'$	$2A + B_2 + B_3$
19	$A_1' + A_1''$	$A + B_3$
20	$A_1' + A_1''$	$A + B_3$
21	$A_1' + A_1''$	$A + B_3$

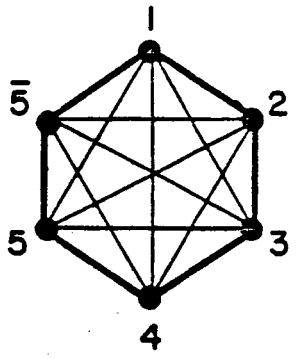

Figure 1. Isomerization reaction graph of the non-rigid molecule Px_2y_2z.

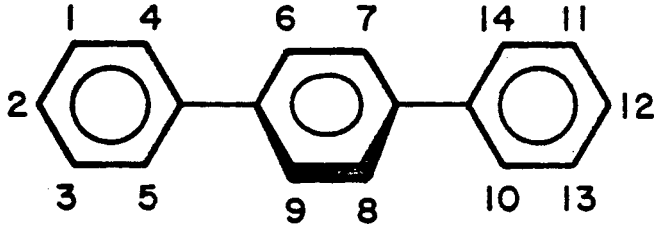

Figure 2. A non-rigid triphenyl molecule. The 21 disubstituted isomers of this molecule are shown in Table 6.

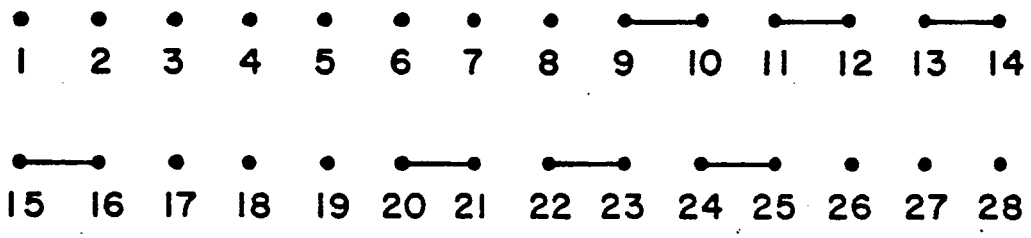

Figure 3. Isomerization reaction graph of a disubstituted non-rigid triphenyl.

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