AJMS
Asian Journal of Mathematical Sciences

RESEARCH ARTICLE

ISOMERS AND PERMUTATIONAL ISOMERIZATION PROCESSES DERIVED FROM TRIGONAL BIPYRAMIDAL MOLECULES; CYCLE INDICES APPROACH

*** JANE RIMBERIA**

Mathematics and Actuarial Science Department, Kenyatta University, P. O. Box 43844-00100, Nairobi, Kenya

Corresponding Email: rimberia.jane@ku.ac.ke

Received: 12-07-2026; Revised: 13-08-2026; Accepted: 28-09-2026

ABSTRACT

The cycle index of a permutation group was introduced by Redfield in 1927, but he called it the group reduction function (Grf). Po'lya independently rediscovered the same function in 1937 and used it to count graphs and chemical compound via the famous Po'lya Enumeration Theorem. Through this theorem, the cycle index became a very powerful tool in enumeration. In this paper, we determine the number of isomers and possible permutational isomerization processes derived from trigonal bipyramidal molecules using Redfield – Po'lya Theorem and Redfield – Read Superposition Theorem. Results show that there are 9 distinct stereoisomers of molecules of the form $MX_iY_jU_k$ and 20 of the type MABCDE. Furthermore, 400 isomerization processes were derived from the trigonal bipyramidal molecule of the type MABCDE.

Keywords: Cycle index, isomers, isomerization processes

INTRODUCTION

Cycle indices are foundational tools in enumerative combinatorics and representation theory. They encode the permutation properties of group actions into structured polynomials, used to count non-equivalent structures such as graphs and chemical isomers and to study the probabilistic properties of groups and random matrices. Several researchers have used cycle indices in enumeration; (See Balasubramanian [1], De Bruijn and Klarner [2], Fugita [3], Gainer-Dewar and Gessel [4], Harary [5]) and Matamala [9]. Now, if a finite group G acts on a set X with n elements, each $g \in G$ corresponds to a permutation σ of X, which can be written uniquely as a product of disjoint cycles. If σ has α_1 cycles of length 1, α_2 cycles of length 2,…, α_n cycles of length n, we say that σ and hence g has cycle type $(\alpha_1, \alpha_2, \ldots, \alpha_n)$. If $g \in G$ has cycle type $(\alpha_1, \alpha_2, \ldots, \alpha_n)$, we define the monomial of g to be $mon(g) = s_1^{\alpha_1} s_2^{\alpha_2} \ldots s_n^{\alpha_n}$, where $s_1, s_2, \ldots, s_n$ are distinct commuting indeterminates. The cycle index of the action of G on X is the polynomial (say over the rational field $\mathbb{Q}$) in $s_1, s_2, \ldots, s_n$ given by

$$Z(G)=\frac{1}{|G|}\sum_{g\in G}\{mon(g)\}\ .\ \text{(Krishnamurthy [7])}$$

If *G* has conjugacy classes $K_1,K_2,\ldots,K_m$ with $g_i \in K_i$, then

$$Z(G)=\frac{1}{|G|}\sum_{i=1}^{m}|K_i|mon(g_i).$$

1. **Preliminaries**

Definition 1.1 (Molecule)

In this paper, a molecule will be regarded as consisting of a skeleton on which there are various sites, with one ligand occupying each site.

Definition 1.2 (Isomers)

They are chemically distinguishable compounds which share the same chemical formula.

Definition 1.3 (Stereoisomers)

They are compounds distinguishable by virtue of the fact that the 3-dimensional arrangement of their constituents differs.

Definition 1.4 (Permutational Isomerization)

Under appropriate conditions, one isomer may transform into another in the process called isomerization. The end result of many isomerization is equivalent to that which would be obtained by simply permuting the positions of the ligands amongst the sites. Such isomerizations are often termed as permutational isomerizations.

Definition 1.5 Weight Function

If a group G acts on a set D, then a weight function on D is simply a map $W:D\to A$ (where A is a suitable algebraic structure) with the property that W is constant on each orbit. The W (d)'s can be thought of as independent variables and polynomial expressions in them with □ -coefficients can be manipulated formally like polynomials. The weight W (ω) of an orbit ω is defined as the weight of any element in it and the sum of the orbit weights is called pattern inventory (PI).

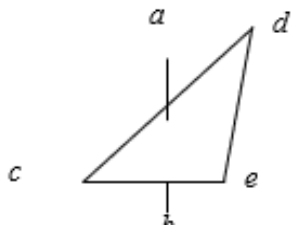
1. **Applications of Redfield – Po'lya Theorem in Enumeration of Isomers of Trigonal Bipyramidal Molecules**

Theorem 2.1: (Redfield – Po'lya Theorem) (Lloyd [8]).

Let D and R be finite sets. Consider the set $R^D=\{f:D\to R\}$ of functions from D to R. Let G be a group of permutations acting on D. Then the action of G on D induces an action of G on R^D given by $g:f\to fg$, where fg is defined by $(fg)(d)=f(g(d))$. Furthermore, if $W:R\to A$ is a weight function and $W(f)=\prod_{d\in D}W(f(d))$, then the pattern inventory (PI) in the action of G on R^D is obtained by substituting $s_i=\sum_{r\in R}(W(r))^i$ into the cycle index of G acting on D.

2.1.1 Stereoisomers of a ML5 complex with three types of ligands X, Y and U

This type of compound has a central metal atom surrounded by five ligands which, in this sub-section, are assumed to be positioned in space like vertices of a regular trigonal bipyramid.



Let $D=\{a,b,c,d,e\}$ and let G be the rotation group of a regular trigonal bipyramid acting on its vertices. Then G consists of the following rotations;

i. Identity.
ii. Rotations through angles $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$ about the vertical axis.
iii. 3 rotations through the angle π about each of the 3 axis passing through the equatorial sites.

The permutations of the five vertices induced by these rotations are as shown in Table 3.1 below.

Table 2.1: Permutations induced by rotations of a trigonal bipyramid

Permutation	**Cycle type**	**Monomial**
1	(5,0,0,0,0)	s_1^5
$(a)(b)(cde)$	(2,0,1,0,0)	$s_1^2 s_3$
$(a)(b)(ced)$	(2,0,1,0,0)	$s_1^2 s_3$
$(e)(ab)(cd)$	(1,2,0,0,0)	$s_1 s_2^2$
$(d)(ab)(ce)$	(1,2,0,0,0)	$s_1 s_2^2$
$(c)(ab)(de)$	(1,2,0,0,0)	$s_1 s_2^2$

Hence the cycle index of G is given by

$$Z(G)=\frac{1}{6}\left(s_1^5+2s_1^2s_3+3s_1s_2^2\right). \qquad (3.1)$$

Let $R=\{X,Y,U\}$ and let $W(X)=X$, $W(Y)=Y$ and $W(U)=U$. Then

$$s_i=\sum_{r\in R}\left(W(r)\right)^i=X^i+Y^i+U^i.$$

Using Theorem 2.1,

$$PI=\frac{1}{6}\left[(X+Y+U)^5+2(X+Y+U)^2\left(X^3+Y^3+U^3\right)+3(X+Y+U)\left(X^2+Y^2+U^2\right)^2\right].$$

By
expansion and simplification we obtain,

$$PI = X^5 + 2X^4Y + 2X^4U + 3X^3Y^2 + 4X^3YU + 3X^3U^2 + 3X^2Y^3 + 6X^2Y^2U + 6X^2U^2Y + 3X^2U^3 + 2XY^4 + 4XY^3U + 6XY^2U^2 + 4XU^3Y + 2XU^4 + Y^5 + 2Y^4U + 3Y^3U^2 + 3Y^2U^3 + 2YU^4 + U^5.$$

The interpretation of the above polynomial expression is that, the coefficient of $X^iY^jU^k$ is equal to the number of stereoisomers of the form $MX_iY_jU_k$. Thus we have;

i. 1 stereoisomer of a MX_5 complex.
ii. 2 stereoisomers of a MX_4Y complex.
iii. 2 stereoisomers of a MX_4U complex.
iv. 2 stereoisomers of a MY_4U complex.
v. 3 stereoisomers of a MX_3Y_2 complex.
vi. 3 stereoisomers of a MX_3U_2 complex.
vii. 3 stereoisomers of a MY_3U_2 complex.
viii. 4 stereoisomers of a MXY_3U complex.
ix. 6 stereoisomers of a MX_2Y_2U complex, with the same number of stereoisomers when *X*, *Y* and *U* are interchanged.

2.1.2 Stereoisomers of a trigonal bipyramidal molecule of the form MABCDE

We substitute

$s_i = \sum_{r \in R} (W(r))^i = A^i + B^i + C^i + D^i + E^i$ in Equation 3.1 to obtain,

$$PI = \frac{1}{6}\left[\begin{matrix}(A+B+C+D+E)^5 + 2(A+B+C+D+E)^2(A^3+B^3+C^3+D^3+E^3) + 3(A+B+C+D+E) \\ (A^2+B^2+C^2+D^2+E^2)^2\end{matrix}\right].$$

On expansion we obtain,

$$\text{Pattern term} = \frac{1}{6}(24ABCDE) \times 5$$

$$= 20\,ABCDE.$$

Hence the molecule has 20 stereoisomers.

2.1.3 Examples on enumeration of stereoisomers of a trigonal bipyramidal molecule

a) Stereoisomers of Iodotricarbonyl(triphenylphoshine) – cobalt (1) complex, $\left[CoI(CO)_3P(C_6H_5)_3\right]$

This complex is of the form MXY_3U. It has a trigonal bipyramidal geometry (Heck [6]). Thus from Subsection 3.1.1, the complex has 4 stereoisomers whose respective drawings are;

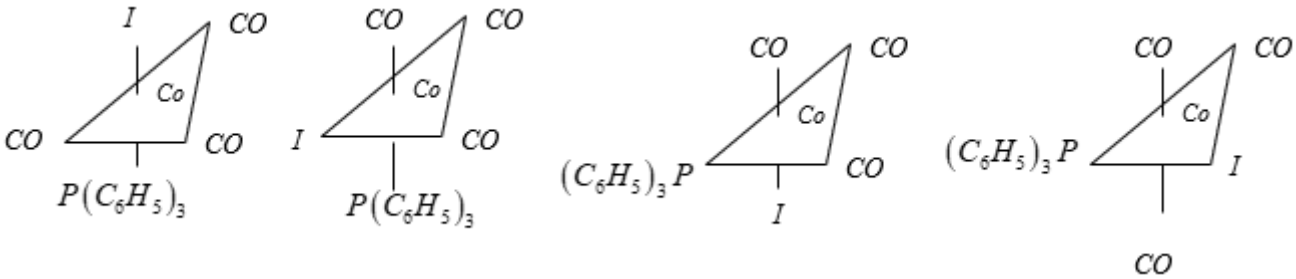


Figure 2: Stereoisomers of Iodotricarbonyl(triphenylphoshine) – cobalt (1) complex

b) Stereoisomers of Hydridocarbonylethylene(bis – triphenylphosphine) – rhodium (1) complex, $\left[RhHCO\left(P\left(C_6H_5\right)_3\right)_2 C_2H_4\right]$

The complex is of the form $MXYU_2V$. It has a trigonal bipyramidal geometry; (Heck [6]). Therefore we substitute

$s_i = \sum_{r\in R}\left(W(r)\right)^i = X^i + Y^i + U^i + V^i$ in Equation 3.1 to obtain,

$$PI = \frac{1}{6}\left[\left(X+Y+U+V\right)^5 + 2\left(X+Y+U+V\right)^2\left(X^3+Y^3+U^3+V^3\right) + 3\left(X+Y+U+V\right)\left(X^2+Y^2+U^2+V^2\right)^2\right].$$

On expansion we obtain,

$$\text{Pattern term} = \frac{1}{6}\left(12\,XYU^2V\right)\times 5$$

$$= 10\,XYU^2V.$$

Hence the complex has 10 stereoisomers.

iv. Enumeration of Permutational Isomerization Processes using Redfield – Read Superposition Theorem

An *n*-ligand molecule may be represented by a 2 x *n* matrix which has site labels in the first row and ligand labels in the second row with $col\left(S_i, L_j\right)$ indicating that site S_i is occupied by ligand L_j. Often the set of the sites has a non-trivial symmetry group *A* associated with it and unless all the ligands are different from one another, there will be a non-trivial ligand symmetry group *B*.

Thus the problem of counting stereoisomers may be tackled by determining the number of orbits of matrices under the combined actions of:

i) The symmetric group S_n permuting intact columns.
ii) The site group A acting on elements in the first row.
iii) The ligand group *B* acting on elements in the second row.

An isomerization process of an *n*-ligand molecule may be represented by a 3 x *n* matrix with $col\left(S_i, L_j, S_k\right)$ indicating that ligand L_j is in site S_i before isomerization and in site S_k afterwards. To obtain an analogue to the above, we allow the group *A* to act on the first row as well as the third row.

Redfield (1927) considered $q\times n$ arrays with S_n permuting intact columns and a group G_i permuting row i $\left(i=1,2,\ldots,q\right)$ and called each row a range and each array a range correspondence. Redfield's group reduced distributions (Grd) and group reduction functions (Grf) are, in modern terminology, the orbits of the arrays under the double action of S_n and $G_1\times G_2\times\ldots\times G_q$ and cycle indices respectively.

Theorem 3.1: (Redfield – Read Superposition Theorem) (Lloyd [8]).

The number of group reduced distributions arising from double action of S_n and $G_1 \times G_2 \times \ldots \times G_q$ on $q \times n$ arrays is equal to

$$N\left(Grf\left(G_1\right) * Grf\left(G_2\right) * \ldots * Grf\left(G_q\right)\right),$$

where $N(P)$ denotes the sum of the coefficients in the polynomial P and the binary operation $*$ is defined as

RULE 1: For identical monomials

$$s_1^{j_1} s_2^{j_2} * s_1^{j_1} s_2^{j_2} = 1^{j_1} j_1! 2^{j_2} j_2! s_1^{j_1} s_2^{j_2} \ldots$$

RULE 2: If $\left(j_1, j_2, \ldots\right) \neq \left(k_1, k_2, \ldots\right)$, then

$$s_1^{j_1} s_2^{j_2} * s_1^{k_1} s_2^{k_2} = 0$$

RULE 3: The composition extends to general polynomials by linearity.

3.1 Examples on enumeration of isomerization processes of trigonal bipyramidal molecules

a) Permutational isomerization processes of Iodotricarbonyl(triphenylphosphine) – cobalt (1) complex, $\left[CoI\left(CO\right)_3 P\left(C_6H_5\right)_3\right]$

This is a trigonal bipyramidal complex of the form MXY_3U, hence the group reduction function of the site group A is given by Equation 3.1.

Since there is 1 ligand of the first type, 3 of the second type and 1 of the third type, the ligand group $B = S_1 \times S_3 \times S_1$.

The group reduction function of a direct product is just the product of group reduction functions of the factors, hence

$$Grf(B) = Grf(S_1) \cdot Grf(S_3) \cdot Grf(S_1).$$

$$\text{Since } S_3 = \left\{1, (123), (132), (12), (13), (23)\right\},$$

$$Grf(S_3) = \frac{1}{6}\left(s_1^3 + 2s_3 + 3s_1 s_2\right) \text{ and so,}$$

$$Grf(B) = \frac{1}{6} \cdot (s_1)^2 \left(s_1^3 + 2s_3 + 3s_1 s_2\right)$$

$$= \frac{1}{6}\left(s_1^5 + 2s_1^2 s_3 + 3s_1^3 s_2\right).$$

Now,

$$Grf(A) * Grf(B) * Grf(A) = \frac{1}{6}\left(s_1^5 + 2s_1^2 s_3 + 3s_1 s_2^2\right) * \frac{1}{6}\left(s_1^5 + 2s_1^2 s_3 + 3s_1^3 s_2\right) * \frac{1}{6}\left(s_1^5 + 2s_1^2 s_3 + 3s_1 s_2^2\right)$$

$$= \frac{1}{216}\left[\left(1^5 5!\right)^2 s_1^5 + 2 \cdot 2 \cdot 2\left(1^2 2! 3^1 1!\right)^2 s_1^2 s_3\right].$$

Hence by Theorem 4.1, the number of theoretically possible permutational isomerization processes of the complex is,

$$N\left(Grf(A)*Grf(B)*Grf(A)\right)=\frac{1}{216}(14400+288)$$
$$=68.$$

b) Permutational isomerization processes of Hydridocarbonylethylene(bis–triphenylphosphine) – rhodium (1) complex, $\left[RhHCO\left(P\left(C_6H_5\right)_3\right)_2C_2H_4\right]$

It is a trigonal bipyramidal complex of the form $MXYU_2V$, hence *Grf*(*A*) is given by equation 2.1.

The ligand group $B=S_1\times S_1\times S_2\times S_1$ and so

$$Grf(B)=Grf(S_1)\cdot Grf(S_1)\cdot Grf(S_2)\cdot Grf(S_1).$$

$S_2=\{1,(12)\}$ and so $Grf(S_2)=\frac{1}{2}\left(s_1^2+s_2\right).$

Therefore

$$Grf(B)=\frac{1}{2}\cdot(s_1)^3\left(s_1^2+s_2\right)$$
$$=\frac{1}{2}\left(s_1^5+s_1^3s_2\right).$$

Now,

$$Grf(A)*Grf(B)*Grf(A)=\frac{1}{6}\left(s_1^5+2s_1^2s_3+3s_1s_2^2\right)*\frac{1}{2}\left(s_1^5+s_1^3s_2\right)*\frac{1}{6}\left(s_1^5+2s_1^2s_3+3s_1s_2^2\right)$$
$$=\frac{1}{72}\left(1^5 5!\right)^2 s_1^5.$$

Therefore by Theorem 4.1, the number of theoretically possible permutational isomerization processes of the complex is,

$$N\left(Grf(A)*Grf(B)*Grf(A)\right)=\frac{1}{72}(14400)$$
$$=200.$$

c) Permutational isomerization processes of a trigonal bipyramidal molecule of the type *MABCDE*

The group reduction function of the site group *A* is given by Equation 3.1. The ligand group $B=S_1\times S_1\times S_1\times S_1\times S_1$, hence

$$Grf(B)=\left(Grf(S_1)\right)^5=s_1^5.$$

Now,

$$Grf(A)*Grf(B)*Grf(A)=\frac{1}{6}\left(s_1^5+2s_1^2s_3+3s_1s_2^2\right)*s_1^5*\frac{1}{6}\left(s_1^5+2s_1^2s_3+3s_1s_2^2\right)$$
$$=\frac{1}{36}\left(1^5 5!\right)^2 s_1^5.$$

Hence by Theorem 4.1, the number of theoretically possible permutational isomerization processes of the complex is,

$$N\left(Grf(A)*Grf(B)*Grf(A)\right)=\frac{1}{36}(14400)$$
$$=400.$$

CONCLUSION

Results show that there are 9 distinct stereoisomers of molecules of the form $MX_iY_jU_k$ and 20 of the type MABCDE. In particular, Hydridocarbonylethylene(bis – triphenylphosphine) – rhodium (1) complex, $\left[RhHCO\left(P\left(C_6H_5\right)_3\right)_2C_2H_4\right]$ was shown to have 10 stereoisomers. Furthermore, 400 isomerization processes were derived from the trigonal bipyramidal molecule of the type MABCDE. For Iodotricarbonyl(triphenylphosphine) – cobalt (1) complex $\left[CoI\left(CO\right)_3P\left(C_6H_5\right)_3\right]$, 68 processes were derived while those for Hydridocarbonylethylene(bis–triphenylphosphine) – rhodium (1) complex, $\left[RhHCO\left(P\left(C_6H_5\right)_3\right)_2C_2H_4\right]$ were 200.

REFERENCES

1. Balasubramanian, K. (1979). Enumeration of stable stereo and position isomers of poly substituted alcohols. Annals New York Acad. Sc. 319(1): 33 – 36. https://doi.org/10.1111/j.1749-6632.1979.tb32771.x

2. De Bruijn, N. G. and Klarner, D. A. (1969). Enumeration of generalized graphs. Koninkl. Nederl. Akad. Van Wet., Pro. Ser. A 72 (1): 1 – 9. https://doi.org/10.1016/1385-7258(69)90020-1

3. Fujita, S. (1990. Enumeration of non-rigid molecules by means of unit subduced cycle indices. Theoretica chimica acta. 77: 307-321. https://doi.org/10.1007/BF01120131

4. Gainer-Dewar, A and Gessel, I.M. (2013). Enumeration of Bipartitite graphs and bipartite blocks. The Electronic Journal of Combinatorics, 1(2) #P2.40. https://doi.org/10.37236/3254
5. Harary, F. (1955). The number of linear, directed, rooted and connected graphs. Transactions of the American Mathematical Society. 78: 445 – 463. https://doi.org/10.1090/S0002-9947-1955-0068198-2

6. Heck, R. F. (1974). Organo transition metal Chemistry. Academic Press, Inc. (London). ISBN 10: 0123361508, ISBN 13: 9780123361509

7. Krishnamurthy, V. (1985). Combinatorics, Theory and Applications, Affiliated East – West Press Private Limited, New Delhi. ISBN-10: 8185336024, ISBN-13: 978-8185336022

8. Lloyd, E. K. (1988). Redfield's papers and their relevance to counting isomers and isomerizations, Discrete Appl. Math. 19: 289 – 304. https://doi.org/10.1016/0166-218X(88)90020-0

9. Matamala, A. (2002). Polya's Combinatorial method and the isomer enumeration problem. Bol. Soc. Chil. Quim. 47: 105-112. http://dx.doi.org/10.4067/S0366-16442002000200006

10. Po'lya, G. (1937). Combinatorial enumeration of groups, graphs and chemical compounds. Acta Math. 68: 145 – 254.
https://doi.org/10.1007/BF02546665

11. Redfield, J. H. (1927). The Theory of group-reduced distributions, J. Amer. Math. Soc. 49:433 – 455.
https://doi.org/10.2307/2370675