

## **A note on Pólya enumeration theory\***

**Werner Hässelbarth**

Institut für Quantenchemie, Freie Universität Berlin, Holbeinstrasse 48 1000 Berlin 45

The power group method of de Bruijn and Harary in enumeration under group action of mappings between finite sets is extended to include correlation of group actions on domain and range. By relaxing the restriction of weight functions to be constant over orbits, more specific results concerning the enumeration of orbits by weight are obtained.

**Key words:** Pólya enumeration theory—power group theorem—Burnside's lemma—symmetry types of mappings—correlation of symmetries

This note deals with what is today called Pólya Enumeration Theory, i.e. the body of material centered about Pólya's famous theorem [1] and its generalizations by de Bruijn [2], Harary [3, 4] and many others. More specifically, it is concerned with an extension of the power group enumeration theorem that was introduced by de Bruijn [2] and further elaborated by Harary and Palmer [3], who coined its name as well. Pólya's theorem enumerates the orbits of mappings between finite sets with respect to a group of permutations on their domain. This setting is generalized in power group enumeration by introducing, besides the domain group, also a group of permutations on the range, which then additionally reduces the number of distinct patterns (orbits). However, this generalization is of a very special type, since the groups of domain and range act jointly but independently of each other, i.e. there is no correlation between the symmetries of domain and range. From the viewpoint of a "chemical combinatorics" it is rather more natural to consider, instead of two such permutation groups, a single point group, say, that acts on the domain and on the range simultaneously. As a consequence, if there is a non-trivial action on both, domain and range, the possibility of some correlation between these actions emerges quite naturally. The present paper

\* This paper is dedicated to Professor Dr. Ernst Ruch on the occasion of this 65th birthday

proposes an extension of power group enumeration that includes correlation of symmetries. Moreover it proposes to relax the restriction on weight functions to be constant on any orbit, which is demanded by the “weighted version” of the Cauchy–Frobenius Lemma<sup>1</sup>. Modern presentations of Pólya Enumeration Theory such as [6, 7, 8, 9] almost inevitably employ this version in order to derive generating functions for the numbers of orbits with various prescribed properties. While the restriction mentioned above is not operative in the case of pure domain action, in power group enumeration it has somewhat unpleasant consequences by lumping together objects that one would like to consider separately. We offer an extension of the weighted Cauchy–Frobenius Lemma that admits a much larger class of weight functions. The generating functions that are obtained in this manner provide more specific results concerning the enumeration of orbits by weight, as compared with the conventional approach.

Both these ideas of introducing correlation between group actions on domain and range, and of abandoning constant weight functions are occasionally mentioned in the literature or used for another purpose, as for instance in [10] and [11]. But to the present author’s knowledge they were never implemented in the body of power group enumeration, which then is the intention of this note.

Let us begin with a summary of the basic facts in Pólya Enumeration Theory, presented from the viewpoint of a single group acting on mappings by acting on their domain or both, on domain and range.

A finite group  $G$  is said to act on a finite set  $M$  if the elements of  $G$  act as permutations on  $M$ , more explicitly, if to each  $g \in G$  a permutation  $\sigma_g \in \text{Sym}(M)$  is associated such that the mapping  $\sigma: g \mapsto \sigma_g$  is a homomorphism from  $G$  into  $\text{Sym}(M)$ , the symmetric group of  $M$ . That is

$$\sigma_g \sigma_{g'} = \sigma_{gg'} \quad \text{for any } g, g' \in G. \quad (1)$$

Synonymously,  $M$  affords a *permutation representation* of  $G$ , or  $M$  is a  *$G$ -set*. The action of the group  $G$  induces an equivalence relation on the set  $M$ ,

$$m' \sim m \Leftrightarrow \exists g \in G: m' = \sigma_g(m), \quad (2)$$

due to which this set decomposes into *orbits*, i.e. equivalence classes under group action. For  $m \in M$ , the symbol  $O_G(m)$  will denote the orbit that contains  $m$ , so

$$O_G(m) := \{m' = \sigma_g(m) | g \in G\}. \quad (3)$$

The action of  $G$  associates to each  $m \in M$  a subgroup of  $G$ , its *stabilizer*

$$G_m := \{g \in G | \sigma_g(m) = m\}, \quad (4)$$

which is related to the orbit  $O_G(m)$  by the fact that the *orbit length*  $|O_G(m)|$ , i.e. the number of elements in the orbit, is given by the stabilizer index.

$$|O_G(m)| = \frac{|G|}{|G_m|}. \quad (5)$$

<sup>1</sup> Which is usually, but erroneously, attributed to Burnside, cf. [5]

By the dual construction, a subset of  $M$  is assigned to each group element  $g \in G$ : the set  $M_g$  of its *fixed points*,

$$M_g := \{m \in M \mid \sigma_g(m) = m\}. \tag{6}$$

The numbers of fixed points,  $|M_g|$ , provide the key to the enumeration of orbits through the

**Cauchy–Frobenius lemma.** *The number of orbits of a  $G$ -set equals the average number of fixed points of the group elements.*

$$\text{no. of orbits} = \frac{1}{|G|} \sum_{g \in G} |M_g|. \tag{7}$$

Given some  $G$ -sets as primary objects, various more complicated  $G$ -sets can be built up from them by means of cartesian products, mappings etc. Pólya’s theory [1] deals with one such construction: with a group acting on mappings by acting on their domain. More explicitly, it starts from a  $G$ -set  $P$  and from another finite set  $L$  (without any group action on it), and next considers the set  $L^P$  of all mappings from  $P$  to  $L$ .

$$L^P := \{\varphi \mid \varphi : P \rightarrow L\}. \tag{8}$$

Let  $\pi_g \in \text{Sym}(P)$  denote the permutation by which  $g \in G$  acts on  $P$ . Then

$$g : \varphi \mapsto \varphi \circ \pi_g^{-1} \tag{I}$$

defines an action of  $G$  on  $L^P$ . Here the symbol  $\circ$  is used for the composition of mappings, that is, for a mapping  $\varphi$  and a permutation  $\pi$ ,  $\varphi \circ \pi$  denotes the mappings that takes  $i \in P$  into  $\varphi(\pi(i))$ .

Alternatively, a group may act on mappings by acting on their range. So let  $L$  be a  $G$ -set, with  $\lambda_g \in \text{Sym}(L)$  representing  $g \in G$ , while there is no group action on the domain  $P$ . In this case

$$g : \varphi \mapsto \lambda_g \circ \varphi \tag{II}$$

defines another action of  $G$  on  $L^P$ —which is, however, not so interesting on its own right but rather in combination with the previous one. So let both,  $P$  and  $L$ , be  $G$ -sets on which  $g \in G$  acts as  $\pi_g$  and  $\lambda_g$ , respectively. Then  $G$  acts on  $L^P$  by acting simultaneously on  $P$  and on  $L$  according to

$$g : \varphi \mapsto \lambda_g \circ \varphi \circ \pi_g^{-1}. \tag{III}$$

$G$ -sets of this type were first discussed by de Bruijn [2] who generalized Pólya’s theory by introducing besides a group of permutations on the domain a second group acting on the range. This amounts to restricting the type III representations to groups which are direct products  $G = A \times B$  of two groups  $A$  and  $B$ , where  $A$  acts exclusively on  $L$  while  $B$  acts on  $P$  only, i.e. we have

$$\begin{aligned} \lambda_{(a,b)} &= \lambda_a \\ \pi_{(a,b)} &= \pi_b \end{aligned} \quad \text{for all pairs } (a, b) \in A \times B, \tag{9}$$

by which the group action on mappings reduces to

$$(a, b): \varphi \mapsto \lambda_a \circ \varphi \circ \pi_b^{-1}. \quad (10)$$

Looking at  $A$  and  $B$  as representing symmetries of range and domain, respectively, there is no correlation between these symmetries in the direct product  $A \times B$ , since any  $a \in A$  combines with any  $b \in B$  into an element  $(a, b)$  of the “similarity group”  $G = A \times B$ . In chemical applications, however, one often encounters a situation where the symmetries of range and domain are correlated, as e.g. when dealing with derivatives of an achiral parent compound where the substituents are allowed to be chiral [12]. A short digression to this subject may be appropriate since counting derivatives of symmetrical parent compounds is the standard application of Pólya Enumeration Theory to “chemical combinatorics”, which we also had in mind when choosing the letters  $P$  and  $L$  to denote domain and range of mappings instead of  $D$  and  $R$ .

For this purpose, let  $P = \{1, 2, 3, \dots\}$  denumerate the *positions* (sites), where substitution may take place in a given parent compound, and let  $L = \{A, B, C, \dots\}$  be a collection of *ligand types* (types of substituents). Mappings from  $P$  to  $L$  obviously represent distributions of ligands of types in  $L$  over the sites of the molecular skeleton in question, if  $\varphi(i) = X$  is taken to say that there is a ligand of type  $X$  at site  $i$ . Let the skeleton have a non-trivial symmetry, and denote by  $G$  the corresponding point-symmetry group, by  $R$  its subgroup of proper rotations, and by  $S$  the coset of improper rotations and reflections. Of course,  $S$  need not exist, namely if the skeleton is chiral. In this setting, one readily identifies symmetry equivalent distributions, that are mutually transformed by proper rotations  $r \in R$ , to represent the same derivative. If, moreover, enantiomers need not be distinguished, mutual transforms by improper rotations  $s \in S$  are identified as well. Evidently, covering operations of the (spatially fixed) skeleton permute the distributions. Moreover, on any distribution, the effect of two consecutive covering operations is the same as that of their product (by the very definition of composition for point-symmetry operations). So the group  $G$  acts on the set  $L^P$  of distributions, and derivatives are orbits with respect to its subgroup  $R$ , while a  $G$ -orbit represents either a mirror image pair of chiral derivatives or an achiral compound.

There are now several possibilities, of increasing complexity, of how this action looks like in detail. First and foremost, a covering operation acts on distributions by removing the ligands from their original positions to other sites, i.e. by permuting the positions of the ligands. Note that this site permutation is the same for all distributions, irrespectively of the kind of ligands that are moved. If the ligand symmetry is sufficiently high, this rearrangement will be the only effect. Otherwise it may happen that a covering operation, besides moving the ligands, also changes their types. For instance, improper rotations and reflections take any chiral ligand into its mirror image—wherever it is situated. Finally, and most awkwardly to deal with, the fate of a ligand may depend on its initial and final position, as will be the case if a ligand type has to be considered a chiral one at some sites and an achiral one at others. Let us now translate these descriptions

of covering operations acting on distributions into definitions of how a group  $G$  acts on a set  $L^P$  of mappings. This is conveniently done by describing the image  $\varphi'$  of a general mapping  $\varphi \in L^P$  under a general group element  $g \in G$ .

First,  $G$  acts through site permutations exclusively. So there is a permutation representation of  $G$  on  $P$ ,  $g \mapsto \pi_g$ , and  $g \in G$  acts on  $\varphi \in L^P$  through taking to site  $\pi_g(i)$  whatever ligand type  $X \in L$  is assigned to  $i \in P$  by the mapping  $\varphi$ . The image  $\varphi'$  is therefore given by  $\varphi'(\pi_g(i)) = X$  if  $\varphi(i) = X$ , equivalently

$$\begin{aligned}\varphi'(i) &= \varphi(\pi_g^{-1}(i)), \quad \text{or} \\ \varphi' &= \varphi \circ \pi_g^{-1}\end{aligned}\tag{11}$$

as a shorthand notation. Second,  $G$  acts on the ligands as well, irrespectively of their position. So a permutation representation of  $G$  on  $L$ ,  $g \mapsto \lambda_g$ , is operative in addition, and  $g \in G$  acts on  $\varphi \in L^P$  by taking to  $\pi_g(i)$  the image  $X = \varphi(i)$  of  $i$  under  $\varphi$ , while transforming it into  $\lambda_g(X)$ . This amounts to  $\varphi'(\pi_g(i)) = \lambda_g(X)$  if  $\varphi(i) = X$ , equivalently,

$$\begin{aligned}\varphi'(i) &= \lambda_g(\varphi(\pi_g^{-1}(i))), \quad \text{or} \\ \varphi' &= \lambda_g \circ \varphi \circ \pi_g^{-1}.\end{aligned}\tag{12}$$

Third, and last, there is an individual<sup>2</sup> permutation representation of  $G$  on  $L$ ,  $g \mapsto \lambda_g^{(i)}$ , for any site  $i \in P$ , and  $g \in G$  takes  $X = \varphi(i)$  into  $\lambda_g^{(i)}(X) = \varphi'(\pi_g(i))$ , i.e.

$$\varphi'(i) = \lambda_g^{(i)}(\varphi(\pi_g^{-1}(i))).\tag{13}$$

The most simple action next to that by pure site permutation occurs in the case of derivatives of an achiral parent compound, where the ligands are allowed to be chiral (but sufficiently symmetric with respect to proper rotations). The proper rotations  $r \in R$  exclusively permute the positions, while improper rotations and reflections  $s \in S$  moreover take any chiral ligand into its mirror image. That is, the point-symmetry group  $G$  acts as follows

$$g: \varphi \mapsto \lambda_g \circ \varphi \circ \pi_g^{-1},\tag{14}$$

where the  $\pi_g$  are the usual site permutations, and where  $\lambda_r = \varepsilon$ , the identity permutation, for all  $r \in R$ , and  $\lambda_s = \tau$ , the product of transpositions ( $XX^*$ ) of mirror image ligand types  $X$  and  $X^*$ , for all  $s \in S$ . Of course we assume that  $X^*$  is in  $L$  if  $X$  is.

The two permutation groups

$$\begin{aligned}\Gamma &= \{\varepsilon, \tau\} \\ \Pi &= \{\pi_g | g \in G\}\end{aligned}\tag{15}$$

represent symmetries of the ligand collection, and of the molecular skeleton, respectively. Their uncorrelated combination would be the direct product group

$$\Gamma \times \Pi = \{(\tau^n, \pi_g) | n = 1, 2; g \in G\},\tag{16}$$

<sup>2</sup> The same for all sites in an orbit of  $P$

acting on  $L^P$  according to

$$(\tau^n, \pi_g): \varphi \mapsto \tau^n \circ \varphi \circ \pi_g^{-1}. \quad (17)$$

The relevant “similarity group” is, however, a subgroup of  $\Gamma \times \Pi$ , that arises from introducing some correlation between the direct factors  $\Gamma$  and  $\Pi$ , namely by eliminating the pairs  $(\varepsilon, \pi_s)$  and  $(\tau, \pi_r)$ .

As a final remark, correlation of symmetries was first implemented in the double coset approach to permutational isomerism at the occasion of dealing with chiral ligands [12]. The consequence then is, that double cosets are replaced by classes of a more general type, the “bilateral classes” introduced in [13], cf. [14] for a recent review.

For evaluating the Cauchy-Frobenius Lemma on the number of orbits, in a permutation representation of one of the types discussed above, the numbers of fixed points of group elements are needed. When  $G$  acts on  $L^P$  via acting on  $P$ ,

$$g: \varphi \mapsto \varphi \circ \pi_g^{-1}, \quad (18)$$

a map  $\varphi$  is invariant under  $g$  if and only if  $\varphi$  is constant on each cyclic factor of the permutation  $\pi_g$ . Hence there are

$$|L|^{c(\pi_g)} \quad (19)$$

fixed points of  $g \in G$  in  $L^P$ , where  $c(\pi_g)$  denotes the number of cycles that appear in the disjoint cycle decomposition of  $\pi_g$  (including the cycles of length one, which are usually omitted!) As a result, the number of  $G$ -orbits in  $L^P$  is

$$\frac{1}{|G|} \sum_{g \in G} |L|^{c(\pi_g)}. \quad (20)$$

When  $G$  acts on mappings by simultaneously acting on domain and range,

$$g: \varphi \mapsto \lambda_g \circ \varphi \circ \pi_g^{-1}, \quad (21)$$

the condition for a map to be a fixed point of some group element is slightly more involved:  $\varphi$  is invariant under  $g$  if and only if  $\varphi$  maps  $k$ -cycles of  $\pi_g$  to fixed points of  $\lambda_g^k$ , the  $k$ -th power of  $\lambda_g$ , in a coherent fashion. Explicitely, let  $i \in P$  be contained in a  $k$ -cycle (cycle of length  $k$ ) of  $\pi_g$ , and let  $\varphi(i) = X$ . Then  $X$  has to be a fixed point of  $\lambda_g^k$ ,  $\lambda_g^k(X) = X$ . Moreover, if  $j$  appears in the same cycle, at the  $\nu$ th position after  $i$ , say, i.e. if  $j = \pi_g^\nu(i)$ , then  $\varphi(j) = \lambda_g^\nu(X)$ . It follows that  $g \in G$  has

$$\prod_{k \geq 1} c_1(\lambda_g^k)^{c_k(\pi_g)} \quad (22)$$

fixed points in  $L^P$ , where  $c_k(\cdot)$  denotes the number of  $k$ -cycles in the cycle decomposition of the permutation in question. Therefore, the number of orbits is given by

$$\frac{1}{|G|} \sum_{g \in G} \prod_{k \geq 1} c_1(\lambda_g^k)^{c_k(\pi_g)}. \quad (23)$$

In the case of type I representations, fairly more detailed information can be obtained from Pólya's theorem. There, the set  $L^P$  is subdivided into classes of mappings having the same *content*, which are then separately decomposed into orbits. The content of a mapping assigns to each element of the range its number preimages in the domain. Formally, for a mapping  $\varphi$  from  $P$  to  $L$ , its content is a function  $J_\varphi$  from  $L$  to the non-negative integers, defined by putting

$$J_\varphi(X) = \text{no. of } i \in P \text{ such that } \varphi(i) = X \quad (24)$$

for any  $X \in L$ . In the case of mappings from the set of substitution positions of a parent compound to a set of substituent types, the content is just the same as the gross formula of derivatives. Evidently, the content of mappings from  $P$  to  $L$  is invariant under site permutations  $\pi \in \text{Sym}(P)$ . Hence it is, of course, invariant under the action of any group  $G$  via site permutations. Therefore, all the subsets of  $L^P$  for the various possible contents are  $G$ -subsets, i.e. they are closed with respect to the action of  $G$ , which makes them  $G$ -sets themselves. Pólya's theorem then gives the number of orbits for any such  $G$ -subset in terms of a single generating function.

**Theorem (Pólya).** *Let a group  $G$  act on  $L^P$  via site permutations, and let  $J$  be a content<sup>3</sup>. Then the number of orbits of mappings with content  $J$  coincides with the coefficient of the monomial*

$$\prod_{X \in L} X^{J(X)} \text{ in the polynomial } \frac{1}{|G|} \sum_{g \in G} \prod_{k \geq 1} \left( \sum_{X \in L} X^k \right)^{c_k(\pi_g)},$$

where the same symbols are used to denote ligand types as well as "indeterminates" assigned to them.

The customary derivation of this famous result employs the so-called "weighted" version of the Cauchy–Frobenius Lemma. For this purpose, the notion of a weight function  $w$  on a set  $M$  is introduced as a mapping  $w: M \rightarrow W$  from  $M$  to some set  $W$  of weights. We shall wish to add weights as well as to divide them by positive integers. So  $W$  has to be closed with respect to addition and multiplication with positive rationals. In practice,  $W$  usually is a ring of polynomials with rational coefficients. Now suppose that  $M$  is a  $G$ -set, and let  $w: M \rightarrow W$  be a weight function that is constant on any orbit of  $M$ . Then it makes sense to call the constant value of the elements in an orbit  $O$  the weight  $w(O)$  of this orbit. In this setting the Cauchy–Frobenius Lemma is readily generalized to the

**Lemma (C.–F., weighted).** *The sum of the orbit weights is the same as the average weight sum of fixed points,*

$$\sum_O w(O) = \frac{1}{|G|} \sum_{g \in G} \sum_{m \in M_g} w(m).$$

<sup>3</sup> I.e. a function  $J$  from  $L$  to the non-negative integers, such that  $\sum_{X \in L} J(X) = |P|$

Specifying to  $M = L^P$ , and to the weight function

$$w(\varphi) = \prod_{i \in P} \varphi(i) = \prod_{X \in L} X^{J_\varphi(X)}, \quad (25)$$

that assigns to a map the product of its images, including multiplicity, results in the following expression for the weight sum of fixed points of  $g \in G$ , acting through a site permutation  $\pi_g$ .

$$\prod_{k \geq 1} \left( \sum_{X \in L} X^k \right)^{c_k(\pi_g)} \quad (26)$$

On the other hand, obviously

$$\sum_O w(O) = \sum_J n_J \prod_{X \in L} X^{J(X)}, \quad (27)$$

where the right hand sum runs over all the possible contents functions, and with  $n_J$  denoting the number of orbits of mappings with content  $J$ . The Pólya Theorem then follows immediately.

Somewhat more generally, one considers weight functions on  $L^P$  that arise from weight functions on  $L$  by assigning to a map  $\varphi: P \rightarrow L$  the product of weights of its images. Explicitly, let  $\omega$  be a weight function on  $L$ , and let  $\hat{X}$  denote the weight  $\omega(X)$  of  $X \in L$  in order to simplify the notation. Assuming that these objects can be added and multiplied commutatively,  $\omega$  is used to construct a weight function  $w$  on mappings,

$$w(\varphi) = \prod_{i \in P} \widehat{\varphi(i)} = \prod_{X \in L} \hat{X}^{J_\varphi(X)}. \quad (28)$$

Then Pólya's theorem takes the slightly more general form of

$$\sum_O w(O) = \frac{1}{|G|} \sum_{g \in G} \prod_{k \geq 1} \left( \sum_{X \in L} \hat{X}^k \right)^{c_k(\pi_g)}. \quad (29)$$

Following de Bruijn [2, 6], we may now proceed in exactly the same manner in order to derive analogous generating functions for orbit numbers when the group  $G$  acts on  $L$  as well. However, the weighted Cauchy–Frobenius Lemma presupposes weight functions to be constant on the orbits of mappings. So, if we stick to the multiplicative weight functions (28)—which is usually done for several reasons<sup>4</sup>— $w$  being constant on orbits of mappings requires  $\omega$  to be constant on orbits of ligand types. So we must have  $\hat{Y} = \hat{X}$  whenever  $Y = \lambda_g(X)$  for some  $g \in G$ . As a consequence, the resulting generating function does not provide the same detail of information as Pólya's. This will be apparent from the example below. Summing up the fixed point weights and invoking the weighted Cauchy–

<sup>4</sup> Multiplicative weight functions provide useful classifications of mappings, and they are nicely handled in computations



Frobenius Lemma results in the following

**Theorem (de Bruijn)**

$$\sum_O w(O) = \frac{1}{|G|} \sum_{g \in G} \prod_{k \geq 1} \left( \sum_{\substack{X \in L \\ \lambda_g^k(X) = X}} \hat{X}^k \right)^{c_k(\pi_g)}$$

As noted before, the original result of de Bruijn<sup>5</sup> is restricted to direct product groups  $G = A \times B$ , where  $A$  acts on  $L$  while  $B$  acts on  $P$ .

Let us apply this result to the derivatives of an achiral parent compound, where the ligands are allowed to be chiral, that were so extensively discussed before. Then  $G$  is again the full point symmetry group of the skeleton in question,  $R$  and  $S$  denote its subgroup of proper rotations, and the coset of improper rotations and reflections, respectively.  $G$  acts on  $L^P$  by

$$g: \varphi \mapsto \lambda_g \circ \varphi \circ \pi_g^{-1}, \tag{30}$$

where  $\lambda_r = \varepsilon$ , the identity permutation, for proper rotations  $r \in R$ , and  $\lambda_s = \tau$ , the overall inversion of chiral ligand types, for the improper symmetry operations  $s \in S$ .  $R$ -orbits of  $L^P$  correspond to derivatives, while  $G$ -orbits either represent mirror image pairs of chiral derivatives or single achiral compounds, depending on whether both the two  $R$ -orbits that are contained in any  $G$ -orbit, are disjoint or identical. Let  $A_1, A_2, \dots, A_i, \dots$  denote the types of achiral ligands, while  $C_1, C_1^*, C_2, C_2^*, \dots, C_j, C_j^*, \dots$  denote the chiral ones, where  $C_j, C_j^*$  is a mirror image pair. Then

$$\tau = \prod_j (C_j C_j^*). \tag{31}$$

The weight function  $\omega$  on  $L$ ,  $\omega(X) = \hat{X}$ , has to take the same value for mirror images. So we put

$$\widehat{C_j^*} = \widehat{C_j}. \tag{32}$$

The right hand side of the expression in de Bruijn's theorem then takes the form

$$\frac{1}{|G|} \left[ \sum_{r \in R} \prod_{k \geq 1} \left( \sum_i \hat{A}_i^k + 2 \sum_j \hat{C}_j^k \right)^{c_k(\pi_r)} + \sum_{s \in S} \prod_{k \geq 2}^{(\text{even})} \left( \sum_i \hat{A}_i^k + 2 \sum_j \hat{C}_j^k \right)^{c_k(\pi_s)} \prod_{k \geq 1}^{(\text{odd})} \left( \sum_i \hat{A}_i^k \right)^{c_k(\pi_s)} \right]. \tag{33}$$

Let  $\alpha_1, \alpha_2, \dots, \alpha_i, \dots$ , and  $\gamma_1, \gamma_2, \dots, \gamma_j, \dots$  be non-negative integers adding up to  $|P|$ . Then the coefficient of the monomial

$$\prod_i \hat{A}_i^{\alpha_i} \prod_j \hat{C}_j^{\gamma_j} \tag{34}$$

in the previous expression (33), after performing all these multiplications and collecting terms, gives the number of achiral derivatives and of mirror image

<sup>5</sup> Called Power Group Enumeration Theorem by Harary and Palmer

chiral pairs, containing  $\alpha_i$  ligands of type  $A_i$  and  $\gamma_j$  ligands of type  $C_j$  or  $C_j^*$ . This type of content, however, lumps together orbit numbers that one should like to (and can, in fact!) have separately. Consider, for a simple example, only one type of chiral ligand  $C$  and its mirror image  $C^*$  at four sites. So  $\alpha_i = \gamma_j = 0$  except for  $\gamma_1 = 4$ , say. The weight  $\hat{C}^4$  comprises five distinct gross formulas

$$C^4, C^3C^*, C^2C^{*2}, CC^{*3}, C^{*4}. \quad (35)$$

However, the mappings of content  $C^2C^{*2}$  constitute a proper  $G$ -set by themselves. Likewise, the mappings of content  $C^3C^*$  form a  $G$ -set together with those of content  $CC^{*3}$ , and the same applies to the contents  $C^4$ ,  $C^{*4}$ . In other words, racemic (i.e. achiral) gross formulas and enantiomeric (i.e. mirror image chiral) pairs of gross formulas define proper  $G$ -sets of which one should like to know the orbit number individually.

In this simple case, these numbers are readily obtained as follows. If a derivative is achiral, its gross formula is necessarily racemic. So we have

$$\begin{aligned} z_G(C^4/C^{*4}) &= z_R(C^4) = z_R(C^{*4}), \\ z_G(C^3C^*/CC^{*3}) &= z_R(C^3C^*) = z_R(CC^{*3}), \end{aligned} \quad (36)$$

where  $z_G(\cdot)$  denotes the number of  $G$ -orbits for the content(s) in question, and the same meaning of  $z_R(\cdot)$ . But we still need

$$z_G(C^2C^{*2}) = ? \quad (37)$$

Now we use the number  $z_G(\hat{C}^4)$ , that the generating function (33) gives us, and from the trivial fact that

$$z_G(\hat{C}^4) = z_G(C^4/C^{*4}) + z_G(C^3C^*/CC^{*3}) + z_G(C^2C^{*2}) \quad (38)$$

the missing orbit number is obtained as

$$z_G(C^2C^{*2}) = z_G(\hat{C}^4) - z_R(C^4) - z_R(C^3C^*). \quad (39)$$

This method of recovering the missing information by means of restricting the group action to subgroups, however, gets quite cumbersome in more complicated cases. So it would certainly be better if all these numbers could be obtained from a single generating function like in Pólya's theorem. This can be done by relaxing the restriction to constant weight functions.

For weight functions that are constant on the orbits of a  $G$ -set  $M$ , the weighted Cauchy-Frobenius Lemma states that

$$\sum_O w(O) = \frac{1}{|G|} \sum_{g \in G} \sum_{m \in M_g} w(m), \quad (40)$$

where we have used the shorthand notation  $gm$  for the image  $\sigma_g(m)$  of  $m \in M$  under  $g \in G$ . Suppose now that  $w$  is not constant on the orbits  $O$ . Then, what replaces the left hand side in (40)? Let  $\Delta$  denote (what  $W$  denoted before; reader, please forgive!) the range of  $w$ , i.e. the set of weights, and for  $\delta \in \Delta$  denote by

$M^{(\delta)}$  its fibre in  $M$ , that is

$$M^{(\delta)} := \{m \in M \mid w(m) = \delta\}. \tag{41}$$

Then the average sum of fixed point weights turns out to be

$$\frac{1}{|G|} \sum_{g \in G} \sum_{\delta \in \Delta} \sum_{\substack{m \in M_g \\ w(m) = \delta}} w(m) = \frac{1}{|G|} \sum_{g \in G} \sum_{\delta \in \Delta} \delta |M_g^{(\delta)}| = \sum_{\delta \in \Delta} \delta \frac{1}{|G|} \sum_{g \in G} |M_g^{(\delta)}|, \tag{42}$$

where  $M_g^{(\delta)}$  denotes the set of fixed points of  $g$  in the fibre  $M^{(\delta)}$ . So the left hand side of what replaces (40) is a linear combination of the weights, with the coefficient of  $\delta \in \Delta$  given by the average number of fixed points in  $M^{(\delta)}$ . In case that  $w$  is constant on the orbits of  $M$ , the subsets  $M^{(\delta)}$  are  $G$ -sets, each, to which the Cauchy-Frobenius Lemma can be applied, resulting in

$$\frac{1}{|G|} \sum_{g \in G} |M_g^{(\delta)}| = \text{no. of orbits in } M^{(\delta)}. \tag{43}$$

From this, the weighted Cauchy–Frobenius Lemma is recovered. But what is the average number of fixed points in an arbitrary subset  $N$  of  $M$ , which is then not a  $G$ -set, as a rule?

$$\begin{aligned} \frac{1}{|G|} \sum_{g \in G} |N_g| &= \frac{1}{|G|} \sum_{n \in N} |G_n| = \sum_{n \in N} \frac{|G_n|}{|G|} \\ &= \sum_{n \in N} \frac{1}{|O_G(n)|} = \sum_{O \in G[N]} \frac{|N \cap O|}{|O|}. \end{aligned} \tag{44}$$

Here  $G_n$  denotes the stabilizer of  $n$ , and the first line is due to the fact that both the first two sums  $\sum |N_g|$  and  $\sum |G_n|$  count the number of pairs  $(g, n)$  such that  $gn = n$ . The final sum runs over the orbits in  $G[N]$ , the closure of  $N$  with respect to  $G$ . In other words,  $G[N]$  is the smallest  $G$ -subset of  $M$  wherein  $N$  is contained.

Suppose now that  $N$  contains the same fraction of all the orbits in  $G[N]$ , that is

$$\frac{|N \cap O|}{|O|} = \text{const. for any } O \text{ in } G[N]. \tag{45}$$

Then we have

$$\sum_{O \in G[N]} \frac{|N \cap O|}{|O|} = \text{const.} \times \text{no. of orbits in } G[N]. \tag{46}$$

For  $n \in N$ , the fraction referring to the orbit  $O_G(n)$  is given by

$$\frac{|N \cap O_G(n)|}{|O_G(n)|} = \frac{1}{|G|} \times \text{no. of } g \in G \text{ such that } gn \in N. \tag{47}$$

So the condition (45) states that the number of group elements leaving  $n \in N$  inside of  $N$  has to be the same for any  $n \in N$ . With reference to a fibre  $M^{(\delta)}$ , this condition then is, that the number of  $g \in G$  such that  $w(gm) = w(m)$  has to be constant on  $M^{(\delta)}$ .

This is automatically true if  $\Delta$  is a  $G$ -set as well, and if  $w: M \rightarrow \Delta$  is a  $G$ -map, that is, if

$$w(gm) = gw(m) \quad (48)$$

holds for any  $g \in G$ ,  $m \in M$ . Here we use the same shorthand notation as before, denoting by  $g\delta$  the image of a weight  $\delta \in \Delta$  under  $g \in G$ . So let  $w$  be a  $G$ -map onto the  $G$ -set  $\Delta$ . Then

$$w(gm) = w(m) \Leftrightarrow gw(m) = w(m) \quad (49)$$

i.e. the number of  $g \in G$  such that  $w(gm) = w(m)$  reduces to the stabilizer order

$$|G_\delta| \text{ for any } m \in M^{(\delta)}, \quad (50)$$

and the constant ratio in (45) turns out to be

$$\frac{|G_\delta|}{|G|} = \frac{1}{|O_G(\delta)|}. \quad (51)$$

Moreover, the closures of fibres are given by

$$G[M^{(\delta)}] = \{m \in M \mid w(m) \in O_G(\delta)\}. \quad (52)$$

Summarizing, we have obtained a generalization of the weighted Cauchy-Frobenius Lemma.

**Lemma (C.-F., generalized weighted version).** *Let  $M$  be a  $G$ -set, and let  $w: M \rightarrow \Delta$  be a weight function such that the number of  $g \in G$  with  $w(gm) = w(m)$  is constant on each of the fibres  $M^{(\delta)}$ ,  $\delta \in \Delta$ . Denote these constant numbers by  $z(\delta)$ . Then*

$$\frac{1}{|G|} \sum_{g \in G} \sum_{m \in M_g} w(m) = \sum_{\delta \in \Delta} a(\delta) \delta,$$

where the coefficients are given by

$$a(\delta) = \frac{z(\delta)}{|G|} \times \text{no. of orbits in } G[M^{(\delta)}].$$

*In particular, let  $\Delta$  be a  $G$ -set as well, and let  $w$  be a  $G$ -map. Then the coefficients  $a(\delta)$  are constant on the orbits of  $\Delta$ . For any such orbit  $\Omega$ , and a weight  $\delta \in \Omega$ ,*

$$a(\delta) = \frac{1}{|\Omega|} \times \text{no. of orbits in } w^{-1}[\Omega],$$

where  $w^{-1}[\Omega]$  denotes the set of  $m \in M$  with  $w(m) \in \Omega$ .

So, also in this quite more general situation, the coefficient of a weight in the average sum of fixed point weights, provides us with an orbit number. We apply this result to type III actions, where a group  $G$  acts on a set  $L^P$  of mappings by acting on domain and range simultaneously,

$$g: \varphi \mapsto \lambda_g \circ \varphi \circ \pi_g^{-1}. \quad (53)$$

As before, we make use of the elements in  $L$  as indeterminates, as well, and we assign to each map  $\varphi: P \rightarrow L$  its gross formula monomial

$$w(\varphi) = \prod_{i \in P} \varphi(i) = \prod_{X \in L} X^{J_\varphi(X)}, \tag{54}$$

where  $J_\varphi$  is the content of  $\varphi$ , i.e.  $J_\varphi(X)$  is the number of sites  $i \in P$  such that  $\varphi(i) = X$ . This weight function  $w$  is readily seen to be a  $G$ -map to the set of monomials over  $L$ , where  $G$  acts according to

$$g: \prod_{X \in L} X^{n(X)} \mapsto \prod_{X \in L} \lambda_g(X)^{n(X)}. \tag{55}$$

Alternatively,  $\varphi \mapsto J_\varphi$  is a  $G$ -map to the set of functions from  $L$  to the nonnegative integers, where  $G$  acts by

$$g: J \mapsto J \circ \lambda_g^{-1}. \tag{56}$$

Now we have to evaluate the generating function

$$\frac{1}{|G|} \sum_{g \in G} \sum_{\substack{\varphi \in L^P \\ \text{fixed by } g}} w(\varphi). \tag{57}$$

This is quite easily done by making use of the previous characterization of fixed points (from which the expression (22) for the fixed point numbers was derived), and of the very same interchange of sum and product that does the job in proving Pólya's theorem. In the appendix we show how to rearrange the sum of fixed point weights into the form

$$\sum_{\substack{\varphi \in L^P \\ \text{fixed by } g}} \prod_{i \in P} \varphi(i) = \prod_{k \geq 1} \left( \sum_{\substack{X \in L \\ \lambda_g^k(X) = X}} \prod_{\nu=1}^k \lambda_g^\nu(X) \right)^{c_k(\pi_g)}. \tag{58}$$

It displays the fact that  $g$ -invariant mappings are constructed cycle-by-cycle, by mapping the sites in each cycle of  $\pi_g$  to a specific set of ligands in a coherent fashion. The sum over the fixed points of  $\lambda_g^k$  enumerates the possible images for cycles of length  $k$ , while the product over all the cycles accounts for the compositions of these partial mappings. This formula is probably due to de Bruijn [11], who used it for quite a different purpose, namely to enumerate the Pólya patterns that are invariant with respect to a prescribed permutation of the ligand types. Let us now define a *generalized gross formula* to be an orbit of monomials over  $L$ . Analogously, a *generalized content* is an orbit of content functions on  $L$ . Both these notions are equivalent, of course, in the sense that

$$\prod_{X \in L} X^{J(X)}, \prod_{X \in L} X^{K(X)}, \dots \tag{59}$$

is an orbit of monomials if and only if

$$J, K, \dots \tag{60}$$

constitute an orbit of content functions. These orbits are the natural substitute of gross formulas, when the group in question acts on the ligands as well, since

the content of mappings in an orbit ranges precisely over an orbit of contents. Putting together the notion of generalized contents, the expression (58) for the sum of fixed point weights, and our generalization of the weighted Cauchy-Frobenius Lemma, results in the following

**Theorem (generalized power group enumeration).** *Let a group  $G$  act on  $L^P$  by acting on  $P$  and  $L$  simultaneously, and let  $\Omega$  be an orbit of content functions on  $L$ . The number of orbits in  $L^P$  with generalized content  $\Omega$  is obtained by summing over all the  $J \in \Omega$  the coefficients of the monomials*

$$\prod_{X \in L} X^{J(X)}$$

in the generating function

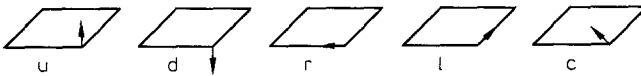
$$\frac{1}{|G|} \sum_{g \in G} \prod_{k \geq 1} \left( \sum_{\substack{X \in L \\ \lambda_g^k(X) = X}} \prod_{\nu=1}^k \lambda_g^\nu(X) \right)^{c_k(\pi_g)}.$$

These coefficients are the same for all the contents  $J \in \Omega$ , so it is sufficient to compute one of them and multiply by  $|\Omega|$ .

Of course, this result can be generalized, in the same manner as the Pólya Theorem, by introducing weights on  $L$ , i.e. by replacing the indeterminates  $X \in L$  by variables  $\hat{X}$  that are allowed to coincide. De Bruijn's theorem is obtained by equating the weights of ligand types within each  $G$ -orbit of  $L$ , which results in

$$\prod_{\nu=1}^k \lambda_g^\nu(X) \text{ being replaced by } \hat{X}^k. \tag{61}$$

We will illustrate this enumeration scheme by means of distributions of arrows over the four corners of a square, with the symmetry group  $D_{4h}$ . The arrows may have different lengths, and moreover they may point upward, down, clockwise, counter-clockwise, and to the center, respectively.



For the sake of simplicity, we restrict ourselves to arrows of the same length; so our set of ligand types is  $L = \{u, d, r, l, c\}$ . With the corners of the square labeled clockwise from 1 to 4, the pairs  $(\lambda_g, \pi_g)$  of permutations  $\lambda_g$  on  $L$ , and  $\pi_g$  on  $P = \{1, 2, 3, 4\}$ , by which the group  $G = D_{4h}$  acts on mappings from  $P$  to  $L$  are given in Table 1.

From this table, the generating function for enumerating orbits of mappings by generalized content is readily seen to be

$$\begin{aligned} & \frac{1}{16} [(u + d + r + l + c)^4 + 2(u^4 + d^4 + r^4 + l^4 + c^4) + (u^2 + d^2 + r^2 + l^2 + c^2)^2 \\ & + 2(2ud + 2rl + c^2)^2 + 2(2ud + 2rl + c^2)c^2 + (r + l + c)^4 \\ & + 2(2u^2d^2 + r^4 + l^4 + c^4) + (2ud + r^2 + l^2 + c^2)^2 \\ & + 2(2rl + u^2 + d^2 + c^2)^2 + 2(2rl + u^2 + d^2 + c^2)(u + d + c)^2]. \end{aligned}$$

**Table 1.**

	(1)(2)(3)(4)	(u)(d)(r)(l)(c)
Rotations about the main axis	(1234)	(u)(d)(r)(l)(c)
	(1432)	(u)(d)(r)(l)(c)
	(13)(24)	(u)(d)(r)(l)(c)
	(12)(34)	(ud)(rl)(c)
Rotations about the dihedral axes	(14)(23)	(ud)(rl)(c)
	(13)(2)(4)	(ud)(rl)(c)
	(24)(1)(3)	(ud)(rl)(c)
	(1)(2)(3)(4)	(ud)(r)(l)(c)
The horizontal refl. improper rotations about the main axis	(1234)	(ud)(r)(l)(c)
	(1432)	(ud)(r)(l)(c)
	(13)(24)	(ud)(r)(l)(c)
	(13)(24)	(ud)(r)(l)(c)
The vertical reflections	(12)(34)	(rl)(u)(d)(c)
	(14)(23)	(rl)(u)(d)(c)
	(13)(2)(4)	(rl)(u)(d)(c)
	(24)(1)(3)	(rl)(u)(d)(c)

**Table 2.**

	$D_{4h}$	$D_4$	$D_{4h}$	$D_4$	stabilizer
1. $c^4$	1	1	1	1	$D_{4h}$
2. $u^4, d^4$	1/2	1/2	1	1	$C_{4v}$
3. $r^4, l^4$	1/2	1/2	1	1	$C_{4h}$
4. $c^3u, c^3d$	1/2	1/2	1	1	$C_{4v}$
5. $c^3r, c^3l$	1/2	1/2	1	1	$C_{4h}$
6. $u^3c, d^3c$	1/2	1/2	1	1	$C_{4v}$
7. $r^3c, l^3c$	1/2	1/2	1	1	$C_{4h}$
8. $u^3d, d^3u$	1/2	1/2	1	1	$C_{4v}$
9. $r^3l, l^3r$	1/2	1/2	1	1	$C_{4h}$
10. $u^3r, d^3r, u^3l, d^3l$	1/4	1/2	1	2	$C_4$
11. $r^3u, l^3u, r^3d, l^3d$	1/4	1/2	1	2	$C_4$
12. $c^2u^2, c^2d^2$	1	1	2	2	$C_{4v}$
13. $c^2r^2, c^2l^2$	1	1	2	2	$C_{4h}$
14. $u^2d^2$	2	2	2	2	$D_{4h}$
15. $r^2l^2$	2	2	2	2	$D_{4h}$
16. $u^2r^2, d^2r^2, u^2l^2, d^2l^2$	1/2	1	2	4	$C_4$
17. $c^2ud$	2	3	2	3	$D_{4h}$
18. $c^2rl$	3	3	3	3	$D_{4h}$
19. $c^2ur, c^2dr, c^2ul, c^2dl$	3/4	3/2	3	6	$C_4$
20. $u^2dc, d^2uc$	1	3/2	2	3	$C_{4v}$
21. $r^2lc, l^2rc$	3/2	3/2	3	3	$C_{4h}$
22. $u^2rc, d^2rc, u^2lc, d^2lc$	3/4	3/2	3	6	$C_4$
23. $r^2uc, l^2uc, r^2dc, l^2dc$	3/4	3/2	3	6	$C_4$
24. $u^2dr, d^2ur, u^2dl, d^2ul$	3/4	3/2	3	6	$C_4$
25. $r^2lu, l^2ru, r^2ld, l^2rd$	3/4	3/2	3	6	$C_4$
26. $u^2rl, d^2rl$	3/2	3/2	3	3	$C_{4v}$
27. $r^2ud, l^2ud$	1	3/2	2	3	$C_{4h}$
28. $cudr, cudl$	3/2	3	3	6	$C_{4h}$
29. $clru, clrd$	2	3	4	6	$C_{4v}$
30. $udrl$	3	5	3	5	$D_{4h}$

There are altogether 70 gross formulas that fall into the 30 orbits given in Table 2, in terms of monomials. The other five columns in this table display

- (i) the coefficients of monomials in the generating function for  $G = D_{4h}$
- (ii) the same for  $R = D_4$
- (iii) the numbers of  $D_{4h}$ -orbits
- (iv) the numbers of  $D_4$ -orbits
- (v) the stabilizers of monomials, to be used only later.

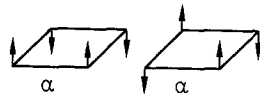
There are, altogether, 61 orbits with respect to  $D_{4h}$ , and 90 for  $D_4$ , as is readily confirmed by means of eqns. (23) and (20).

$$\frac{1}{16}[5^4 + 2 \cdot 5 + 5^2 + 2 \cdot 5^2 + 2 \cdot 5 + 3^4 + 2 \cdot 5 + 5^2 + 2 \cdot 5^2 + 2 \cdot 5 \cdot 3^2] = 61, \quad (63)$$

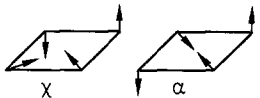
$$\frac{1}{8}[5^4 + 2 \cdot 5 + 5^2 + 2 \cdot 5^2 + 2 \cdot 5] = 90.$$

Let us check these results by drawing some pictures, where we make use of the fact that any  $G$ -orbit either contains two mirror image chiral  $R$ -orbits or a single

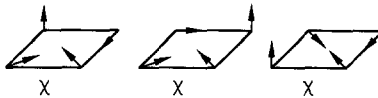
14.  $u^2d^2$



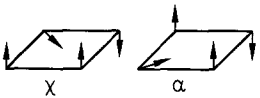
17.  $c^2cd$



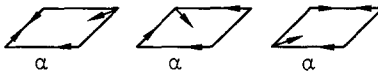
19.  $c^2ur, \dots$



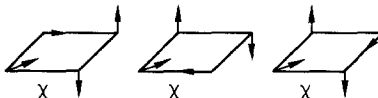
20.  $u^2dc, \dots$



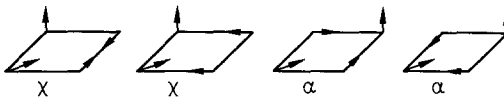
21.  $r^2lc, \dots$



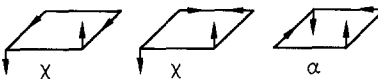
28.  $cudr, \dots$



29.  $ciru, \dots$



30.  $udrl$





achiral one. So we will list, for some selected general contents, representatives of the  $G$ -orbits, and by classifying them to be either achiral ( $\alpha$ ) or chiral ( $\chi$ ), transversals of  $R$ -orbits could be obtained by adding mirror images of the chiral ones.

If one is not so much interested in the complete series of orbit numbers but rather in single such numbers for particular generalized contents, some simplification may be possible. Consider e.g. the set of mappings with generalized content  $\{c^2ur, c^2dr, c^2ul, c^2dl\}$ . By the Cauchy–Frobenius Lemma, the number of orbits in this set equals the average number of fixed points. But the rotations about the main axis are the only elements in  $D_{4h}$ , that can possibly fix a mapping in this set, since the dihedral rotations as well as the improper rotations and reflections do not even fix the content of any such mapping. So, with  $f(g)$  denoting the number of maps fixed by  $g$ ,

$$\begin{aligned} \frac{1}{|D_{4h}|} \sum_{g \in D_{4h}} f(g) &= \frac{1}{|D_{4h}|} \sum_{g \in C_4} f(g) \\ &= \frac{1}{4} \left\{ \frac{1}{|C_4|} \sum_{g \in C_4} f(g) \right\}. \end{aligned} \tag{64}$$

Hence there are four times as many  $C_4$ -orbits as there are orbits with respect to  $D_{4h}$ . Finally, the four contents  $c^2ur, c^2dr, c^2ul, c^2dl$  specify four distinct but equivalent  $C_4$ -sets, and so we end up with the result that there are equally many  $D_{4h}$ -orbits of content  $\{c^2ur, c^2dr, c^2ul, c^2dl\}$  and  $C_4$ -orbits of content  $c^2ur$ , say. The latter number, however, is given by Pólya’s theorem to be the coefficient of  $c^2ur$  in the generating function

$$\frac{1}{4}[(c + u + r)^4 + 2(c^4 + u^4 + r^4) + (c^2 + u^2 + r^2)^2], \tag{65}$$

which then is readily computed to be three. In fact, the following theorem holds

**Theorem.** *Let a group  $G$  act on  $L^P$  by acting on  $P$  and on  $L$  simultaneously. Let  $\Omega$  be a generalized content, i.e. an orbit of content functions, and let  $J \in \Omega$  be one of them. Denote by  $G_J$  its stabilizer. Then the set of mappings with content  $J$  is a  $G_J$ -set, and there are equally many  $G$ -orbits of generalized content  $\Omega$  and  $G_J$ -orbits of content  $J$ .*

In this manner, the generalized contents may be replaced by ordinary ones again, namely by a transversal from the orbits of content functions. The last column in the previous table specifies the stabilizers of contents for our example. Four groups,  $D_{4h}, C_{4v}, C_{4h}$  and  $C_4$  occur, which fix  $c/c, u, d/c, r, l/c, u, d, r, l$  respectively. So we have, for example,

$$\begin{aligned} z_{D_{4h}}(u^2rl, d^2rl) &= z_{C_{4v}}(u^2rl), \\ z_{D_{4h}}(r^2ud, l^2ud) &= z_{C_{4h}}(r^2ud). \end{aligned} \tag{66}$$

Instead of proving the theorem above we wish to present a somewhat stronger result to be used in “constructive combinatorics”, that is, for the purpose of

constructing transversals (systems of representatives) of orbits instead of merely counting them. Let  $M$  and  $N$  be  $G$ -sets, and let  $w: M \rightarrow N$  be a  $G$ -map, i.e. for any  $g \in G, m \in M$

$$w(gm) = gw(m). \quad (67)$$

For any orbit  $B$  of  $N$ , denote by  $w^{-1}[B]$  the set of elements  $m \in M$  with  $w(m) \in B$ ,

$$w^{-1}[B] := \{m \in M \mid w(m) \in B\}. \quad (68)$$

Any such set  $w^{-1}[B]$  is a  $G$ -subset of  $M$ , since  $w(m) \in B$  implies  $w(gm) = gw(m) \in B$ . In case that  $w$  is surjective, all the  $w^{-1}[B]$  are non-empty, and they constitute a decomposition of  $M$  into  $G$ -subsets. Since

$$Jm w := \{n = w(m) \mid m \in M\} \quad (69)$$

is in turn a  $G$ -subset of  $N$ , we may restrict ourselves to this subset, in other words, we can assume  $w$  to be a map onto  $N$ . Accordingly, the decomposition of  $N$  into orbits  $B$  induces a decomposition of  $M$  into  $G$ -subsets  $w^{-1}[B]$ , which then may be decomposed into orbits, separately. Now we observe that, for any orbit  $A$  in  $w^{-1}[B]$ , the images  $w(a)$  of its elements run through  $B$  as  $a$  runs through  $A$ . So any such orbit  $A$  has at least one element in the fibre of an arbitrary  $b \in B$ ,

$$w^{-1}(b) := \{m \in M \mid w(m) = b\}. \quad (70)$$

On the other hand, two such preimages are in the same  $G$ -orbit if and only if they are already in the same  $G_b$ -orbit, where  $G_b$  is the stabilizer of  $b \in B$ . Namely, suppose that  $m$  and  $m'$  are in the same  $G$ -orbit, that is,  $m'$  may be expressed as  $m' = gm$  with some  $g \in G$ . Suppose that  $w(m) = w(m') = b$ . Then it follows from  $b = w(m') = w(gm) = gw(m) = gb$ , that any such  $g \in G$  that takes  $m$  into  $m'$ , has to be in the stabilizer  $G_b$ . Since the fibre  $w^{-1}(b)$  is a  $G_b$ -set, of course, our result may be summarized as follows.

**Theorem.** *Let  $M$  and  $N$  be  $G$ -sets, and let  $w$  be a  $G$ -map from  $M$  onto  $N$ . Let  $B$  be any  $G$ -orbit in  $N$ , and  $b \in B$  an arbitrary element. Then, any transversal from the  $G_b$ -orbits in  $w^{-1}(b)$  is a transversal from the  $G$ -orbits of  $w^{-1}[B]$  as well. In particular, there are as many  $G_b$ -orbits in  $w^{-1}(b)$  as there are  $G$ -orbits in  $w^{-1}[B]$ .*

By means of this result, the decomposition of a given  $G$ -set  $M$  into its orbits can be facilitated, if a  $G$ -map  $w$  onto another  $G$ -set  $N$  is available, and if  $N$  is easier decomposed into orbits as  $M$  is. After computation of a transversal  $T = \{b\}$  from the  $G$ -orbits in  $N$ , as an intermediate step, the fibres  $w^{-1}(b)$  are decomposed into  $G_b$ -orbits, each, and a transversal  $T_b$  is chosen from these orbits. Then

$$\bigcup_{b \in T} T_b \quad (71)$$

is a transversal from the  $G$ -orbits of  $M$ .

As noted before, assigning to a map its content function or its gross formula monomial is a  $G$ -map from  $M = L^P$  to the sets of content functions on  $L$ , and

of monomials over  $L$ , respectively, on which  $G$  acts in the obvious fashion. The previous assertion then follows immediately.

As a final remark, we should like to mention that bilateral classes [13] may be employed in counting “de Bruijn-patterns” in the very same manner as double cosets are used to enumerate “Pólya-patterns” [15]. For the number of bilateral classes, closed form expressions similar to those for double cosets are available, which may then be used instead of generating functions. This can be quite profitable in case that only a few orbit numbers are required.

**Appendix: Evaluation of weighted fixed point sums**

With reference to formula (58) we alluded to a well-known trick which is essential to evaluating sums of fixed points weights for multiplicative weight functions, namely by interchanging summation and multiplication. We will now indicate how such procedures work, in general. For this purpose, let  $A$  and  $B$  be finite sets, and let each  $a \in A$  be associated with a specific weight function  $w_a$  on  $B$ . We assume again that weights can be added and multiplied commutatively. Assign to each map  $\psi$  from  $A$  to  $B$  the product of its images according to

$$\psi \mapsto \prod_{a \in A} w_a(\psi(a)). \tag{72}$$

We wish to evaluate sums of these objects, where we restrict the mappings from  $A$  to  $B$  by assigning to each  $a \in A$  a specific subset  $B_a \subseteq B$  of admissible images. The result then is

$$\sum_{\substack{\psi \in B^A \\ \psi(a) \in B_a}} \prod_{a \in A} w_a(\psi(a)) = \prod_{a \in A} \sum_{b \in B_a} w_a(b). \tag{73}$$

It is quite easily verified by arbitrarily ordering the elements in  $A$ , and by identifying mappings from  $A$  to  $B$  with their tuples of images. Putting  $n = |A|$ ,  $w_i = w_{a_i}$ ,  $B_i = B_{a_i}$ , the previous result is obtained as follows.

$$\begin{aligned} \sum_{\substack{\psi \in B^A \\ \psi(a) \in B_a}} \prod_{a \in A} w_a(\psi(a)) &= \sum_{b_1 \in B_1} \sum_{b_2 \in B_2} \cdots \sum_{b_n \in B_n} w_1(b_1)w_2(b_2) \cdots w_n(b_n) \\ &= \left( \sum_{b_1 \in B_1} w_1(b_1) \right) \left( \sum_{b_2 \in B_2} w_2(b_2) \right) \cdots \left( \sum_{b_n \in B_n} w_n(b_n) \right) \\ &= \prod_{a \in A} \sum_{b \in B_a} w_a(b). \end{aligned} \tag{74}$$

Formula (58) is immediately recovered by choosing

$A =$  collection of cycles of  $\pi_g$

$B = L$

$B_a =$  subset of fixed points of  $\lambda_g^k$ , for cycle length  $k$

$w_a(X) = X\lambda_g(X)\lambda_g^2(X) \cdots \lambda_g^{k-1}(X)$ , for cycle length  $k$ ,

while the Pólya Theorem refers to

$$B_a = B = L, \text{ for any cycle of } \pi_g$$
$$w_a(X) = X^k, \text{ for cycle length } k.$$

*Acknowledgement.* The author wishes to express his thanks to Professor A. Kerber for drawing his attention to the method of generating functions, in stimulating discussions.

## References

1. Pólya, G.: Acta Math. **68**, 145 (1937)
2. de Bruijn, N. G.: Indag. Math. **21**, 59 (1959)
3. Harary, F., Palmer, E.: J. Comb. Theory **1**, 157 (1966)
4. Harary, F.: Am. math. Monthly **66**, 572 (1959)
5. Neumann, P. M.: Math. Scientist **4**, 133 (1979)
6. de Bruijn, N. G.: in Applied combinatorial mathematics, pp. 744, E. F. Beckenbach, ed. New York: Wiley 1964
7. Harary, F., Palmer, E.: Graphical enumeration, New York: Academic Press, 1973
8. Kerber, A.: Representations of permutation groups II, Lecture Notes in Mathematics, Vol. **495**. Berlin: Springer Verlag 1975
9. Kerber, A., in The permutation group in physics and chemistry, pp. 1, Lecture Notes in Chemistry, Vol. **12**. Berlin: Springer Verlag 1979
10. Davidson, R. A.: Ph.D. Thesis, The Pennsylvania State University, 1977
11. de Bruijn, N. G.: J. Comb. Theory **2**, 418 (1967)
12. Hässelbarth, W., Ruch, E.: Israel J. Chem. **15**, 112 (1977)
13. Hässelbarth, W., Ruch, E., Klein, D. J., Seligman, T. H.: J. Math. Phys. **21**, 951 (1980)
14. Ruch, E., Klein, D. J.: Theoret. Chim. Acta (Berl.) **63**, 447 (1983)
15. Ruch, E., Hässelbarth, W., Richter, B.: Theoret. Chim. Acta (Berl.) **19**, 288 (1970)

Received March 12, 1984