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On the interrelation between orbits and double cosets

Werner Hässelbarth

Institut für Quantenchemie, Freie Universität Berlin, Holbeinstraße 48, D-1000 Berlin 45, Federal Republic of Germany

Orbits and double cosets are intimately related: double cosets can always be looked upon as being orbits and often orbits can be identified with double cosets, in reverse. This note presents two such situations where orbits can be traced back to double cosets: the restriction of transitive permutation representations to subgroups and the cartesian product of two transitive permutation representations. These results readily apply to standard topics in chemical combinatorics dealing with isomers and isomerizations but equally like to less familiar combinatorial schemes such as Redfield's.

Key words: Enumeration under group action—orbits—double cosets—permutational isomerism

In a recent contribution [1], McLarnan emphasized the connections between the two current approaches to counting isomers and isomerizations: the method of generating functions à la Pólya and the double coset formalism, as established e.g. in [2-4] and [5-7], respectively. More specifically, he pointed out that double cosets can be looked upon as being orbits. Hence, the Cauchy-Frobenius Lemma¹—which is also basic to the Pólya method—applies to their enumeration, yielding simple proofs of known formulas. The present note intends to shed some further light on the interrelation between double cosets and orbits by means of two simple theorems. They are, in fact, simple enough to be, most probably, folklore among mathematics professionals in enumeration under group action but, to the author's knowledge, they are nowhere recorded in the current literature on this subject.

¹ Usually, but erroneously, attributed to Burnside, cf. [8].

A finite group G is said to act on a finite set M, if the group elements $g \in G$ are associated (homomorphically) with permutations $\pi_g \in \text{Sym}(M)$ of the elements $m \in M$. When abbreviating $\pi_g(m)$ to gm, the homomorphism condition $\pi_g \pi_{g'} = \pi_{gg'}$ takes the form g(g'm) = (gg')m, i.e. there is no need for brackets. Due to the action of G, the set M decomposes into equivalence classes, the orbits $O_G(m)$

$$O_G(m) = \{ m' = gm \mid g \in G \}.$$
⁽¹⁾

Their number, according to the Cauchy-Frobenius Lemma, coincides with the average number of fixed points of the group elements,

no. of orbits =
$$\frac{1}{|G|} \sum_{g \in G} f(g)$$
, (2)

where f(g) denotes the number of $m \in M$ such that gm = m. G is said to act transitively on M if M has only one G-orbit. The final ingredient from the theory of enumeration under group action is the notion of the stabilizer of an element $m \in M$, that is, the subgroup G_m made up by those group elements that fix m,

$$G_m = \{g \in G \mid gm = m\}. \tag{3}$$

Various equivalence classes in a group G such as cosets, double cosets and conjugacy classes may be looked upon as being orbits, due to an action on G of some subgroup of G or of the direct square $G \times G$. So, e.g. right and left cosets Ag, gB arise as orbits of subgroups A and B, acting on G by left and right translations, respectively:

$$a: g \mapsto ag, \tag{4}$$
$$b: g \mapsto gb^{-1}.$$

Another action of subgroups A is that by conjugation,

$$a: g \mapsto aga^{-1},$$
 (5)

which leads to the A-conjugacy classes, in particular to the ordinary conjugacy classes for A = G. Finally, for a direct product $A \times B$ of two subgroups, acting through bilateral translation,

$$(a, b): g \mapsto agb^{-1}, \tag{6}$$

the orbits are the (A, B)-double cosets

$$AgB = \{g' = agb^{-1} \mid a \in A, b \in B\}.$$
(7)

By extending this action to arbitrary subgroups Q of $G \times G$, one arrives at the notion of bilateral classes [9]. Since all these classes are orbits, they can be enumerated through the Cauchy-Frobenius Lemma. In fact, a general formula for the number of bilateral classes is available [9b] which reduces to the expressions for the numbers of (A, B)-double cosets and of A-conjugacy classes, as cited by McLarnan [1] from [5] and [6], by specializing Q to be a direct

product $A \times B$ or the diagonal of a direct square, $(A \times A)_d$,

no. of
$$(A, B)$$
-double cosets $= \frac{|G|}{|A||B|} \sum_{\rho} \frac{|C_{\rho} \cap A||C_{\rho} \cap B|}{|C_{\rho}|}$.
no. of A-conjugacy classes $= \frac{|G|}{|A|} \sum_{\rho} \frac{|C_{\rho} \cap A|}{|C_{\rho}|}$.
(8)

In both these formulas, the sum is over the (ordinary) conjugacy classes C_{ρ} of G.

Now we are ready to introduce the first one of our two folklore theorems, which is about the restriction of transitive permutation representations to subgroups. That is: given a set M on which a group G acts transitively, and a subgroup Hof G, we will describe the H-orbits of M. Since G acts transitively, any $m' \in M$ may be written as an image m' = gm of an arbitrarily fixed $m \in M$ under some $g \in G$. However, this representation is not unique, in general, since g'm = gm if (and only if) g' and g are in the same left coset of the stabilizer G_m , i.e. $g' \in gG_m$. On the other hand g'm and gm are in the same H-orbit if and only if g'm = hgmfor some $h \in H$. Putting both these trivialities together, we arrive at the condition $g' = hgg_m$ where $h \in H$, $g_m \in G_m$ in other words: g' and g are in the same double coset of G with respect to the subgroups H and G_m . So we end up with

Theorem 1. Let a group G act transitively on a set M. Then the orbits of a subgroup H of G are in one-to-one correspondence with the double cosets of G with respect to H and to the stabilizer G_m of an arbitrary element $m \in M$. More explicitly, let T be a transversal² of the double cosets HgG_m . Then $Tm = \{gm | g \in T\}$ is a transversal of the H-orbits in M.

$$G = \bigcup_{g \in T} HgG_m \Leftrightarrow M = \bigcup_{g \in T} O_H(gm).$$

Applications of this result start, the other way around, from an intransitive action of a group H on a set M, looking for a transitive extension to some supergroup G of H. It is quite obvious that such transitive extension need not exist—apart from the possibility of identifying H with its image in Sym(M) and choosing for G a transitive group between Sym(M) and this image, which is as trivial as useless. In concrete cases such as of groups acting on sets of mappings by acting on their domain and their range, one has to be lucky to find a "reasonable" transitive extension. In such fortunate cases, our theorem provides a description of orbits in terms of double cosets, which may be used, e.g., to compute their number, to construct transversals and to investigate their automorphism groups.

Example 1: Pólya patterns and double cosets

Pólya's enumeration theorem [2] refers to groups acting on (sets of) mappings by acting on their respective domains. Explicitly, then, let a finite group G act on a finite set $P = \{1, 2, 3, ..., 2i, ...\}$ through permutations, $g \mapsto \pi_g \in \text{Sym}(P)$.

² "Transversal" is a short form of "system of representatives".

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Then

$$g: \varphi \mapsto \varphi' = \varphi \circ \pi_g^{-1}, \text{ i.e. } \varphi'(i) = \varphi(\pi_g^{-1}(i))$$
(9)

defines an action of G on the set L^P of mappings φ from P to any other set $L = \{A, B, C, \ldots, X, \ldots\}$. Since G acts through permutations of the "sites" $i \in P$, symmetry-equivalent distributions φ and $\varphi' = \varphi \circ \pi_g^{-1}$ of "ligands" in L over the sites in P have the same "gross formula", that is, the frequencies $F_{\varphi}(X) = no$. of $i \in P$ such that $\varphi(i) = X$ are the same for φ and φ' . So we may fix some gross formula F (i.e. a function from L to the non-negative integers such that $\sum F(X) = |P|$ and ask for the number of orbits of G in the subset L_F^P of mappings with this gross formula. Pólya's theorem provides the answer. Alternatively, we may start from the following observation. Let $G^{(P)}$ denote the group of site permutations through which G acts on P, i.e.

$$G^{(P)} = \{ \pi_g \in \operatorname{Sym}(P) | g \in G \}.$$
(10)

Then, trivially, G-orbits and $G^{(P)}$ -orbits in L^P coincide, if we let $G^{(P)}$ act on mappings from P to L according to

$$\pi: \varphi \mapsto \varphi' = \varphi \circ \pi^{-1} \text{ for } \pi \in G^{(P)}.$$
(11)

This action can, of course, be extended to the full symmetric group Sym(P), and then the Sym(P)-orbits in L^P turn out to be just the subsets L_F^P of mappings with some fixed gross formula, since site permutations do not change the gross formula of mappings, and, on the other hand, any two mappings with the same gross formula are mutually convertible by site permutations. Thus we may use the preceding theorem and establish a one-to-one correspondence between the *G*-orbits in L_F^P and the double cosets of Sym(P) with respect to $G^{(P)}$ and the stabilizer of an arbitrarily chosen mapping $\varphi \in L_F^P$. This stabilizer, however, is just the Young-subgroup Y_{φ} associated with φ , i.e. the direct product of the symmetric groups on the homogeneously substituted subsets of P,

$$Y_{\varphi} = \operatorname{Sym}(P_A) \times \operatorname{Sym}(P_B) \times \cdots$$
ere
(12)

where

$$P_X = \{i \in P \mid \varphi(i) = X\}.$$

So we end up with the well-known result [5], that the G-orbits of mappings $\varphi: P \to L$ with gross formula F are in one-to-one correspondence with the double cosets of the symmetric group Sym(P) with respect to the image $G^{(P)}$ of G and an appropriate Young-subgroup Y_{φ} . More precisely, let Y_{φ} be the Young-subgroup of $\varphi \in L_F^P$. Then, if T is a transversal of the double cosets $G^{(P)}\pi Y_{\varphi}$ in Sym(P), $T_{\varphi} = \{\varphi \circ \pi^{-1} | \pi \in T\}$ is a transversal of the G-orbits in L_F^P .

Example 2: Redfield's range correspondences and double cosets

The basic schemes in enumeration under group action, as introduced by Pólya [2] and generalized by de Bruijn [3, 10], Harary and Palmer [11] and many others, are concerned with orbits of mappings between finite sets, under actions of groups

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on domain and range. Another such fundamental scheme - in fact the first one in this field - was laid out by Redfield [12] in 1927. His paper appears to have gone unnoticed until the 1960's when Foulkes [13] and Harary and Palmer [14] directed attention to Redfield's work. More recently, Kerber and Lehmann [15] presented a joint generalization of Pólya's and Redfield's theories, cf. also [16], and Davidson [17] pointed out the utility of Redfield's approach in chemical combinatorics. Redfield's objects are correspondences between the elements of k equicardinal sets called ranges, i.e. k-ary relations of a particular type. The case of k = 3 sets will suffice to illustrate the idea. So let X, Y, Z be three sets, each with n elements $x_1, x_2, \ldots x_n/y_1, y_2, \ldots y_n/z_1, z_2, \ldots z_n$. A matrix of size $3 \times n$,

$$\begin{pmatrix} x_{\pi(1)} & x_{\pi(2)} & \dots & x_{\pi(n)} \\ y_{\sigma(1)} & y_{\sigma(2)} & \dots & x_{\sigma(n)} \\ z_{\tau(1)} & z_{\tau(2)} & \dots & z_{\tau(n)} \end{pmatrix},$$
(13)

where π , σ and τ are permutations of the integers from 1 to *n*, constitutes a correspondence between the elements of X, Y and Z. Evidently, two such matrices induce the same correspondence if and only if they are mutually interconvertible by permuting the columns. So the $(n!)^3$ matrices fall into $(n!)^2$ classes (of size n!, each), one for any correspondence. Now let Q be a subgroup of the direct product of symmetric groups $S_X \times S_Y \times S_Z$. (Here we write S_X as a short form of Sym(X) as well as S_n for the symmetric group of the first *n* natural numbers). That is: Q is a group permuting the elements within each row. Call two matrices row-equivalent (with respect to Q) if they are transformed into each other by an element of Q, column-equivalent in the situation discussed before. Joining both these equivalences, Redfield arrives at what might be called Q-classes of correspondences: his term is "group-reduced distributions". In particular, Redfield shows that if the x_i , the y_i , and the z_i are the nodes of three graphs, and if $Q = G \times H \times K$, where G, H and K are the automorphism groups of the X-graph, the Y-graph and the Z-graph, respectively, then the Q-classes account for the various "superpositions" of these three graphs.

Starting from the preceding description, theorem 1 is readily applied as follows. The direct product $S_X \times S_Y \times S_Z$ acts transitively on the set of correspondences between X, Y, and Z, i.e. on the set of collections of columns

$$\left\{ \begin{pmatrix} x_{\pi(i)} \\ y_{\sigma(i)} \\ z_{\tau(i)} \end{pmatrix} \middle| i = 1, 2, \dots, n \right\},$$
(14)

So what we still need is the stabilizer of an arbitrary such correspondence. We choose

$$\left\{ \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} \middle| i = 1, 2, \dots, n \right\},$$
(15)

which is fixed by the diagonal subgroup

$$(S_X \times S_Y \times S_Z)_d = \{(\pi, \pi, \pi) \mid \pi \in S_n\},\tag{16}$$

and thus we end up with a bijection between the Q-classes of correspondences and the double cosets of $S_X \times S_Y \times S_Z$ with respect to its diagonal and to Q. Turning to enumeration, we make use of the formula (8) for the number of double cosets AgB in G. Identifying S_X , S_Y and S_Z with S_n , the number of Q-classes turns out to be

no. of Q-classes =
$$\frac{|S_n|^2}{|Q|} \sum_{\rho} \frac{|C_{\rho} \times C_{\rho} \times C_{\rho} \cap Q|}{|C_{\rho}|^2},$$
(17)

where the C_{ρ} , this time, denote the conjugacy classes of S_n . If, in particular, Q' is a direct product, say $Q = G \times H \times K$, then

no. of Q-classes =
$$\frac{|S_n|^2}{|G||H||K|} \sum_{\rho} \frac{|C_{\rho} \cap G||C_{\rho} \cap H||C_{\rho} \cap K|}{|C_{\rho}|^2}$$
 (18)

The case of k = 2 sets X and Y deserves some extra attention. Correspondences between two sets are plainly bijections, and Q-classes are orbits of bijections under a group of (more or less correlated) symmetries of their domain and range. Theorem 1 relates them to the double cosets of $S_X \times S_Y$ with respect to its diagonal and to Q. These double cosets may be further reduced to bilateral classes [9] in S_n ,

$$Q[\tau] = \{\tau' = \pi \tau \sigma^{-1} | (\pi, \sigma) \in Q\},\tag{19}$$

in particular to double cosets $G\tau H$, in case that Q is a direct product subgroup, $Q = G \times H$. Formally, this is done by mapping the direct square $S_n \times S_n$ onto S_n according to $(\pi, \sigma) \mapsto \pi \sigma^{-1}$. This mapping takes double cosets of $S_n \times S_n$ with respect to its diagonal (on the right) and another subgroup Q into Q-bilateral classes of S_n by "cancelling" the factor $(S_n \times S_n)_d^3$. On the other hand, Q-classes of bijections are immediately related to bilateral classes in S_n by identifying both the x's and the y's with their labels, which turns bijections between X and Y into permutations of the numbers 1 to n. For further details compare [18] as a recent review of both, double cosets and bilateral classes.

Let us now turn to another relation between orbits and double cosets. It refers to the cartesian product of two transitive permutation representations as follows. If a group G acts on two sets M and N, these two actions naturally combine to a single action of G on the cartesian product $M \times N$

$$g:(m, n) \mapsto (gm, gn). \tag{20}$$

There is no chance for this action to be transitive unless G acts transitively on both, M and N. But even then, their cartesian product $M \times N$ will, in general, decompose into several orbits. These orbits are in one-to-one correspondence with the double cosets of G with respect to the stabilizers G_m and G_n of two arbitrary elements $m \in M$, $n \in N$ as follows: Since G acts transitively on M as

³ Alternatively, this relation between Q-bilateral classes of a group G and double cosets of $G \times G$ with respect to $(G \times G)_d$ and Q is an easy consequence of theorem 1: The supergroup $G \times G$ of Q acts transitively on G, its diagonal is the stabilizer of the identity, hence the double cosets of $G \times G$ with respect to these two subgroups are in one-to-one correspondence with the orbits of Q acting on G, i.e., with the Q-bilateral classes in G.

well as on N, any pair $(m', n') \in M \times N$ can be expressed as a pair of images (g_1m, g_2n) of two fixed elements $m \in M$, $n \in N$ under two appropriate group elements $g_1, g_2 \in G$. Now (g_1m, g_2n) and (g'_1m, g'_2n) are in the same G-orbit if, and only if, there is some $g \in G$ such that $g'_1 \in gg_1G_m$ and, simultaneously, $g'_2 \in gg_2G_n$. This holds precisely if $g'_1^{-1}g'_2 \in G_mg_1^{-1}g_2G_n$. So, our result is

Theorem 2. Let a group G act transitively on two sets M and N. Then the G-orbits of the cartesian product $M \times N$ are in one-to-one correspondence with the double cosets of G with respect to G_m and G_n , the stabilizers of two arbitrary elements $m \in M$, $n \in N$. More precisely, let T be a transversal of the double cosets $G_m gG_n$. Then $\{m\} \times Tn = \{(m, gn) | g \in T\}$ is a transversal⁴ of the G-orbits in $M \times N$.

$$G = \bigcup_{g \in T} G_m g G_n \Leftrightarrow M \times N = \bigcup_{g \in T} O_G((m, gn)).$$

This result could as well be obtained as a corollary to theorem 1 as follows. If G acts transitively on both M and N, then $G \times G$ acts transitively on $M \times N$ according to

$$(g,h):(m,n)\mapsto(gm,hn).$$
(21)

Restriction of this action to the diagonal subgroup $(G \times G)_d$ yields the previous action of G on $M \times N$. The stabilizer of a pair (m, n) is the direct product of the individual stabilizers, $G_m \times G_n$. So, application of theorem 1 results in a one-to-one correspondence between the G-orbits of $M \times N$ and the double cosets of $G \times G$ with respect to its diagonal and the direct product subgroup $G_m \times G_n$. The mapping $(g, h) \mapsto gh^{-1}$ from $G \times G$ onto G, in turn, takes these double cosets $(G \times G)_d(g, h)(G_m \times G_n)$ into the double cosets $G_m gh^{-1}G_n$, in a one-to-one fashion. Of course, this approach is unnecessarily complicated, but it demonstrates the general applicability of theorem 1 (together with one or two more tricks, which may be needed in order to obtain the optimum result).

There is still another road to theorem 2, which starts from the following observation. As before let a group G act on a cartesian product $M \times N$ by acting, componentwise, on M and on N. We wish to compute a transversal from the orbits. So let T be a transversal of the G-orbits in M. Then, if $m_1, m_2 \in T$ are two distinct representatives, pairs (m_1, n_1) and (m_2, n_2) are in different G-orbits in $M \times N$, whatever $n_1, n_2 \in N$ may be. But pairs $(m, n_1), (m, n_2)$ with the same M-component can be in the same G-orbit, namely if (and only if) there is some $g \in G$ which takes n_1 into n_2 while fixing m. So, we have

Lemma. Let a group G act on $M \times N$ by acting on M and on N. Furthermore, let T be a transversal from the G-orbits in M, and, for any $m \in T$, let T_m be a transversal from the G_m -orbits in N. Then $\{(m, n) | m \in T, n \in T_m\}$ is a transversal of the G-orbits in $M \times N$.

In particular, if G acts transitively on M, the G-orbits in $M \times N$ bijectively correspond to the G_m -orbits in N. In case that G acts transitively on N as well,

⁴ Each representative (m, gn) could of course be substituted by any of the pairs (g_1m, g_2n) with $g_1^{-1}g_2 = g$.

we may again invoke theorem 1, resulting in a one-to-one correspondence between the G-orbits in $M \times N$ and the double cosets of G with respect to the stabilizers G_m , G_n of two arbitrary elements $m \in M$, $n \in N$.

As a remark in passing, the preceding lemma is quite interesting on its own right since it provides the basis for an efficient method to construct transversals [19] e.g. in the case of groups acting on (sets of) mappings by acting on their domain.

Example 3: Isomerizations via highly symmetric transition states

In his paper [1], McLarnan discusses rearrangements of molecular or crystal systems from an initial state I with symmetry A to a final state F with symmetry B via some transition state T with symmetry G, such that I and F may be represented as orbits of colorings of T. A and B then are the stabilizers G_i and G_f of some initial and final coloration, and the rearrangements $I \rightarrow T \rightarrow F$ are given by the G-orbits in the cartesian product $I \times F$, i.e. in the set of pairs (i', f') of initial and final colorations. These orbits are, in turn, in one-to-one correspondence with the double cosets AgB in G (or the BgA, equivalently).

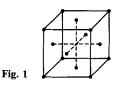
Example 4: Superpositions of Pólya patterns

As in example 1, let a group G act on a set of mappings, L^{P} , by acting on their domain, P. Suppose that P decomposes into two G-orbits, Q and R. Since any mapping from P to L uniquely corresponds to a pair of mappings from Q to Land from R to L, and vice versa, L^{P} may be identified with the cartesian product $L^Q \times L^R$. Trivially, G acts on both factors by acting on Q and on R, and componentwise action coincides with the original action of G on L^{P} . So, instead of decomposing L^P into orbits, we may first decompose L^Q and L^R , separately, and then, for any two orbits, construct their superpositions, by decomposing their cartesian product into orbits. Now let $\varphi \in L^Q$ and $\psi \in L^R$ be two such partial mappings. Then the superpositions of the corresponding patterns, i.e. the orbits in the cartesian product $O_G(\varphi) \times O_G(\psi)$, are in one-to-one correspondence with the double cosets $G_{\varphi}gG_{\psi}$ in G. Explicitly, let T be a transversal of these double cosets. Then $\{(\varphi, \psi \circ \rho_g^{-1}) | g \in T\}$ is a transversal from the orbits of mappings with Q-part in $O_G(\varphi)$ and R-part in $O_G(\psi)$. Here $\rho_g \in \text{Sym}(R)$ is the permutation by which g acts on R, and the pairs $(\varphi, \psi \circ \rho_g^{-1})$ are glued together to form a mapping from P to L according to

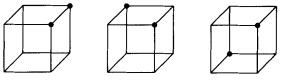
$$(\varphi, \psi \circ \rho_g^{-1}): i \mapsto \begin{cases} \varphi(i) & \text{for } i \in Q\\ \psi(\rho_g^{-1}(i)) & \text{for } i \in R \end{cases}$$
(22)

By iterating this procedure, Pólya Enumeration can be refined to include specification of a partial gross formula for each orbit of sites.

For an explicit example, consider a cubic arrangement of sites, as shown in Fig. 1, i.e. a superposition of a cube and an octahedron.



The corners of the cube as well as those of the octahedron are to be coloured black or white, and we are interested in the orbits of colorations under the octahedral group, with two of the cubic sites and one of the octahedral sites coloured black, the remaining 13 sites coloured white (or simply uncoloured, in our figures). Up to orientation, there are three such partial colorations of the cube,





while there is of course only one for the octahedron.



The stabilizers of these partial colorations are $C_2 = \{e, c_2\}$, $C'_2 = \{e, c_4^2\}$ and D_3 for the cubic ones, and C_4 for the octahedral one. The octahedral group has

- 3 double cosets with respect to C_2 and C_4 ,
- 4 double cosets with respect to C'_2 and C_4 ,
- 1 double coset with respect to D_3 and C_4 .

Indeed, there are three superpositions

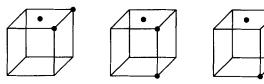
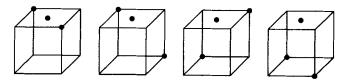


Fig. 4

four of the type



and finally one of the third type.



Fig. 6

It is, of course, no more than an easy exercise to implement this refinement into Pólya's generating function as well. If $P_1, P_2, \ldots, P_{\nu}, \ldots$ are the G-orbits in P, upon which $g \in G$ acts through permutations $\pi_g^{(1)}, \pi_g^{(2)}, \ldots, \pi_g^{(\nu)}, \ldots$, then the result is given by

$$\frac{1}{|G|} \sum_{g \in G} \prod_{\nu} \prod_{k \ge 1} \left(\sum_{X_{\nu} \in L_{\nu}} X_{\nu}^{k} \right)^{a_{k}(\pi_{g}^{(\nu)})}.$$
(23)

In this expression, we use different symbols $X_1, X_2, \ldots, X_{\nu}, \ldots$ to denote the same ligand type X as occurring in the various orbits of sites, and we also attribute individual sets L_{ν} of admissible ligand types to them. In the exponents, $a_k(\cdot)$ stands for the number of cycles of length k of the permutation in question. The coefficient of any monomial

$$\prod_{X_{\nu}} X_{\nu}^{F(X_{\nu})} \tag{24}$$

in the polynomial above gives the number of G-orbits of mappings with $F(X_{\nu})$ ligands of type X on sites in the ν -th orbit of P.

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References

- 1. McLarnan, T. J.: Theoret. Chim. Acta 63, 195 (1983).
- 2. Pólya, G.: Acta Math. 68, 145 (1937)
- 3. de Bruijn, N. G. in: Applied Combinatorial Mathematics, pp. 144, E. F. Beckenbach ed., New York: Wiley, 1964
- 4. (a) Klemperer, W. G.: J. Chem. Phys. 56, 5478 (1972)
 (b) Klemperer, W. G.: Inorg. Chem. 11, 2668 (1972)
 and further contributions by the same author in J. Am. Chem. Soc. (1972/73)
- 5. Ruch, E., Hässelbarth, W., Richter, B.: Theoret. Chim. Acta 19, 288 (1970)
- 6. Hässelbarth, W., Ruch, E.: Theoret. Chim. Acta 29, 259 (1973)
- 7. Klein, D. J., Cowley, A. H.: J. Am. Chem. Soc. 97, 1633 (1975)
- 8. Neumann, P. M.: Math. Scientist 4, 133 (1979)
- 9. (a) Hässelbarth, W., Ruch E., Klein, D. J., Seligman, T. H. in: Group Theoretical Methods in Physics, Proc. V. Int. Colloq. Montreal 1976, Academic Press 1977
 (b) Hässelbarth, W., Ruch, E., Klein, D. J., Seligman, T. H.: J. Math. Phys. 21, 951 (1980)
- 10. de Bruijn, N. G.: Indagationes Math. 21, 59 (1959)
- 11. Harary, F., Palmer, E.: J. Comb. Theory 1, 157 (1966)
- 12. Redfield, J. H.: Am. J. Math. 49, 433 (1927)
- 13. Foulkes, H. O.: Can. J. Math. 18, 1060 (1966)

- 14. Harary, F., Palmer, E.: Am. J. Math. 89, 373 (1967)
- 15. Kerber, A., Lehmann, W.: Match 3, 67 (1977)
- Kerber, A. in: The Permutation Group in Physics and Chemistry, pp. 1, Lecture Notes in Chemistry Vol. 12, Berlin: Springer, 1979
- (a) Davidson, R. A.: J. Am. Chem. Soc. 103, 312 (1981)
 (b) Davidson, R. A.: Generalized Redfield Combinatorics, preprint 1981
- 18. Ruch, E., Klein, D. J.: Theoret. Chim. Acta 63, 447 (1983)
- 19. Hässelbarth, W., Kerber, A., Ruch, E.: Symmetry classes of mappings (in preparation)

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