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An Invitation to Permutation Representations of Groups

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As an analogue of linear group representations, where groups act on vector spaces by linear transformations, the notion of a permutation representation refers to groups acting on finite sets by permuting their elements. There exists a well-developed theory of permutation representations which is, however, practically unknown outside of (but even very little known within) mathematics. The present paper reviews its basic notions and results, and it sketches actual and prospective applications in »chemical combinatorics«, where this theory promises to be of similar value as that of linear representation theory in quantum chemistry.

1. INTRODUCTION

Group representations are realizations of more or less »abstract« groups as subgroups of »concrete« groups. More precisely, a representation of a group G as a subgroup of another group H is a homomorphism of G into H, that is: a mapping $G \ni g \rightarrow h_g \in H$ such that

$$h_g h_{g'} = h_{gg'} \tag{1}$$

holds for any two elements $g, g' \in G$. The images $h_g \in H$ of the $g \in G$ constitute a subgroup of H which provides a (not necessarily faithful) realization of G.

The most important types of »concrete« groups are

i) matrix groups or, equivalently, groups of linear operators such as $H = GL(n, \mathbb{C})$, the group of non-singular complex (nxn)-matrices, or $H = GL(V)$, the group of invertible linear operators of some vector space V,

ii) permutation groups such as $H = \mathrm{Sym}(S)$, the symmetric group of a finite set S, i. e. the group of permutations of its elements.

Representations of the first type are called linear representations; often the attribute »linear« is simply omitted because of the predominance of this type throughout mathematics, physics and chemistry. Representations of the second type are called permutation representations. We take the opportunity to fix some notation while recalling their definition.

A permutation representation of a group G on a finite set S attributes to any group element $g \in G$ a permutation $\pi_g \in \mathrm{Sym}(S)$ such that holds for any $g, g' \in G$. Synonymously, the group G is said to act (as a permutation group) on the set S, and S is called a G — set. Unless there is some danger of confusing different actions of the same group on the same set, we shall write gs as a short form of $\pi_g(s)$, the image of an element $s \in S$ under the permutation π_g by which $g \in G$ acts in the representation in question. Then the homomorphism condition (2) takes the form $g(g's) = (gg')s$, i. e. there is no need for brackets in this notation.

A group action induces an equivalence relation on the set in question.

$$s' \sim s \Longleftrightarrow \exists\ g \in G : s' = gs, \tag{3}$$

due to which this set decomposes into equivalence classes, its orbits with respect to the group action

$$O_G(s) := \{s' = gs \mid g \in G\}. \tag{4}$$

The most immediate questions about orbits refer to their sizes and their number. The answers are equally easy: the size of an orbit is given by the stabilizer index of any element, and the number of orbits equals the average number of fixed points of the group elements. These results involve two dual objects which a group action associates with any element of the set and of the group in question: the stabilizer G_s of an element $s \in S$

$$G_s := \{g \in G \mid gs = s\}, \tag{5}$$

and the set S_g of fixed points of a group element $g \in G$

$$S_g := \{s \in S \mid gs = s\}. \tag{6}$$

The stabilizer G_s is a subgroup of G. Its left cosets are in one-to-one correspondence with the elements in the orbit $O_G(s)$, hence

$$|O_G(s)| = \frac{|G|}{|G_s|}. \tag{7}$$

Turning to the number of orbits, the following observation provides a convenient starting point. Let E be an equivalence relation on a finite set S, and let $E(s)$ denote the equivalence class containing $s \in S$. Then, trivially,

$$\sum_{s' \in E(s)} \frac{1}{|E(s')|} = 1 \tag{8}$$

holds, and therefore the number n of equivalence classes is given by

$$\sum_{s \in S} \frac{1}{|E(s)|} = n. \tag{9}$$

This general identity is, however, totally useless — unless we have sufficient information about the sizes of equivalence classes, as we do if they are orbits under the action of a group. For $E(s) = O_G(s)$, eq. (7) leads to

$$n = \frac{1}{|G|} \sum_{s \in S} |G_s|. \tag{10}$$

Noting finally that

$$\sum_{s \in S} |G_s| = \sum_{g \in G} |S_g|, \tag{11}$$

since both these sums enumerate the pairs (g, s) such that $gs = s$, we arrive at

$$n = \frac{1}{|G|} \sum_{g \in G} |S_g| = \langle f(g) \rangle_{g \in G} \tag{12}$$

where we have introduced $f(g) = |S_g|$ for the number of fixed points of a group element $g \in G$ and brackets for averaging. This result is commonly attributed to Burnside — Burnside's lemma-but it is in fact due to Frobenius and to Cauchy, comp. (*1*).

Symmetric polyhedra provide immediate illustrations of the notions introduced above. Any covering operation of a polyhedron induces a permutation of its corners as well as of its edges, its faces and so on, and the effect of two consecutive operations is the same as that of their product (by the very definition of that product). So e. g. let S be the set of corners of a symmetric polyhedron, and let G be its point-symmetry group. Then G acts on S. The orbits of this action are the subsets of symmetry-equivalent corners, the stabilizer of a corner accounts for its site symmetry, and fixed points are points on the rotation axis for proper rotations, and points in the mirror plane for reflections.

Example 1: A trigonal bipyramid,

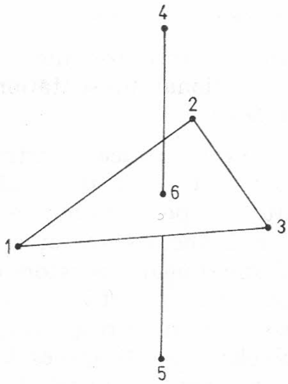

Figure 1

$S = \{1, 2, 3, 4, 5, 6\}$

$G = D_3 = \{e, c_3, c^2_3, c_2, c_2', c_2''\}$

(we restrict ourselves to the proper rotational point-symmetry)

the permutation representation of G:

g	π_g
e	(1) (2) (3) (4) (5) (6)
c_3	(123) (4) (5) (6)
c^2_3	(132) (4) (5) (6)
c_2	(1) (23) (45) (6)
c_2'	(13) (2) (45) (6)
c_2''	(12) (3) (45) (6)

stabilizers: $G_1 = C_2$, $G_2 = C_2'$, $G_3 = C_2''$, $G_4 = C_3$, $G_5 = C_3$, $G_6 = D_3$.

fixed points: $S_e = S$, $S_{c_3} = S_{c_3^2} = \{4, 5, 6\}$, $S_{c_2} = \{1, 6\}$, $S_{c_2'} = \{2, 6\}$, $S_{c_2''} = \{3, 6\}$.

orbits: $\{1, 2, 3\}$, $\{4, 5\}$, $\{6\}$.

The reader may check that indeed the orbit lengths coincide with the stabilizer indices in question, and that three is the average fixed point number of the group elements.

Starting from the notions and results above about groups acting on sets, which are commonplace today, it is an easy matter to proceed along the lines of ordinary (i. e. linear) representation theory, developing a theory of permutation representations. However, these few simple things already have such a wealth of applications that almost nobody cared(s). Various objects throughout mathematics and sciences such as molecules and graphs can be identified with orbits of appropriate groups acting on appropriate sets. Hence Burnside's lemma applies to their enumeration. The best-known example is Polya's theory[2] — certainly the most popular topic in advanced mathematics among chemists. Today a whole branch of combinatorics is devoted to »enumeration under group action«, that is, to the art of applying Burnside's lemma, compare e. g. Harary and Palmer's monograph[3] on the enumeration of graphs.

In the next paragraph, we will review the basic notions and results of the theory of permutation representations, emphasizing analogy with ordinary representation theory. It was created by Burnside roughly a century ago[4], with modern presentations given by Dress[5] and Knutson[6].

2. THE THEORY OF PERMUTATION REPRESENTATIONS

The object of this paragraph is to mimic the linear representation theory of finite groups. We follow the lines of its traditional presentation, which we briefly sketch for the convenience of the reader.

A linear representation of a group G on a vector space V attributes to any group element $g \in G$ a linear operator L_g of V such that $L_g L_{g'} = L_{gg'}$ holds for any $g, g' \in G$. Mimicking the nomenclature of permutation representation theory for the time being, we may call V a G-vectorspace or a G-space, for short, and we may say that G acts on V (by linear operators/transformations). Next, some structure is introduced into the jungle of linear representations of a given group by means of two classification principles: similarity and decomposition into elementary building blocks. Two G-spaces V and V' are called equivalent (i. e. they carry equivalent representations) if they are isomorphic vector spaces, and if, in addition, the isomorphism between them is compatible with the actions of G on V and V', that is: if there is an invertible linear transformation $T: V \rightarrow V'$ such that $TL_g = L'_g T$ holds for any $g \in G$. Turning to decomposition, a subspace W of V is called a G-subspace (invariant subspace) if it is stable under the action of G, that is, if $L_g w \in W$ for any $g \in G$, $w \in W$. Hence a G-space is either reducible or irreducible, meaning that it has some (non-trivial) G-subspace or it hasn't. Due to the fact* that any G-space can be endowed with a G-invariant scalar product, i. e. such that the L_g are unitary operators, any G-space decomposes into a direct sum of irreducible G-subspaces. Synonymously, in any matrix representation, all the representation matrices can be simultaneously transformed into the same block-diagonal shape such that the individual diagonal blocks constitute ir-

* True for finite groups and compact *Lie* groups.

reducible matrix representations. Skipping the important problem of how to effectively perform such decomposition (projection operators, symmetry adapted bases), the notions of equivalence and (ir)reducibility provide an enormous simplification. In studying the representations of a given group, we may restrict ourselves to irreducibles, and it turns out that up to equivalence, there is only a finite number of them for a finite group. Schur's lemma provides the key to their further investigation. Its objects are the G-maps (intertwining maps) between two G-spaces V and V'. These are linear transformations $T: V \rightarrow V'$ that are compatible with the actions of G, compare the definition of equivalence. For given G-spaces V, V', the collection of G-maps from V to V' forms a vector space, and Schur's lemma states that for irreducibles, this intertwining space has dimension one or zero, depending on whether V, V' are equivalent or not. This result is then employed in deriving the »orthogonality relations« among the matrix element functions of irreducible representations, the main computational tool in the calculus of representation theory. Up to equivalence a finite group has as many irreducible representations as conjugacy classes. However, even today, a satisfactory recipe is missing of how to construct a complete set for an arbitrary finite group. There is no such gap in character theory, which is the appropriate tool for studying representations up to equivalence. The character of a representation $(g \mapsto L_g)$ is a function that attributes to any group element $g \in G$ a complex number $\chi(g) = \mathrm{tr} L_g$, the trace of its representation operator (matrix). Two G-spaces are equivalent if and only if their characters coincide. Characters are constant on conjugacy classes, $\chi(g) = \chi(hgh^{-1})$, and the irreducible characters constitute an orthonormal basis in the vector space of functions $f: G \rightarrow \mathbb{C}$ which share this invariance property. As a final ingredient, the character of a reducible representation is the sum of the characters of its irreducible constituents. Hence the multiplicity, up to equivalence again, of an irreducible representation in a reducible one is given by the corresponding scalar product of characters. This fact makes the analysis of representations a matter of simple numerical computations — once the character table of the group in question, i. e. the collection of its irreducible characters, is known. For the point-symmetry groups, the character tables are collected in almost any book on »Group Theory and Applications«. Moreover, there are general methods to compute character tables for arbitrary finite groups, and special receipes for particular families such as the symmetric groups S_n.

These are the basic notions and results of linear representation theory that we are going to mimic, referring to permutation representations. We will also briefly discuss analogues of constructions not reviewed here, such as subduced/induced representations and tensor products.

Turning to permutation representations now, we begin by introducing similarity and fragmentation like before. Two G-sets S and S' are called equivalent, if there is one-to-one correspondence $s \leftrightarrow s'$ between the elements of S and those of S' such that $gs_1 = s_2 \Longleftrightarrow gs_1' = s_2'$. That is, there is a bijection $\varphi: s \mapsto s'$ from S onto S' such that $\varphi(gs) = g\varphi(s)$ for any $g \in G$, $s \in S$. Invariant subsets take the part of invariant subspaces in linear representation theory.

A subset $T \subseteq S$ is called a G-subset, if $gt \in T$ for any $g \in G$, $t \in T$. Thus the action of G may be restricted to T, turning this set into a G-set. A G-set is called simple, if it has no (proper) G-subsets. Synonynously, G is said to act transitively on S. Apparently simple G-sets are the analogues of irreducible G-spaces. There seems to be no standard name for the analogues of reducibles, so we are free to call them composite G-sets; the group action then is intransitive. Any G-set uniquely decomposes into simple constituents: it is the disjoint union of its orbits — parallel to any G-space decomposing (almost uniquely) into a direct sum of irreducibles. Next we look for the analogue of Schur's lemma. In linear representation theory, this key result is due to the fact that for any intertwining map, both its image and its kernel are invariant subspaces of the G-spaces in question. If both these spaces are irreducible, the result then is that there is essentially one interwining map between equivalent spaces and no such map between inequivalent spaces. So our objects are G-maps between G-sets, that is, mappings that are compatible with the actions of G. Formally, a mapping φ: $S \to S'$ from a G-set S into another G-set S' is called a G-map, if $\varphi(gs) = g\varphi(s)$ holds for any $g \in G$, $s \in S$. The image of φ, that is, the collection of images $\varphi(s)$, $s \in S$, constitutes a G-subset of S'. So, if S' is simple, φ must be »onto«. However, the analogue of the kernel is missing, and hence the permutation representation version of Schur's lemma turns out to be not quite as nice as the original one. Unlike in the linear theory, there are G-maps between inequivalent simple G-sets. But we can characterize them all and, more important, we can recognize equivalent simple G-sets.

Lemma: Let S and S' be two simple G-sets. There is a G-map from S to S' if and only if there are elements $s \in S$, $s' \in S'$ such that the stabilizer G_s is contained in $G_{s'}$. In particular, S and S' are equivalent if and only if there are elements $s \in S$, $s' \in S'$ with identical stabilizers, $G_s = G_{s'}$.

Elements within an orbit have mutually conjugate stabilizers,

$$G_{gs} = g\, G_s\, g^{-1}. \tag{13}$$

Hence we may fix two arbitrary elements $s \in S$, $s' \in S'$ and rephrase the lemma as follows.

Lemma': There is a G-map from S to S' if and only if G_s is subconjugate to $G_{s'}$, that is, if some conjugate gG_sg^{-1} is contained in $G_{s'}$. In particular, S and S' are equivalent if and only if G_s and $G_{s'}$ are conjugates.

Still another version makes explicit use of the notion of conjugacy classes of subgroups. Let us introduce the notation $H \leq G$ as a short form of "H is a subgroup of G", and $|H$ for the collection of conjugates of H,

$$IH := \{H' = gHg^{-1} \mid g \in G\}. \tag{14}$$

We also introduce a partial ordering among these conjugacy classes, inherited from the subgroup relation, as follows: $|H \leq |K$ if and only if there are $H' \in |H$, $K' \in |K$ such that $H' \leq K'$, equivalently, if and only if H is subconjugate to K.

If S and S' are simple G-sets, the stabilizers G_s and $G_{s'}$ of their elements range over two conjugacy classes of subgroups; let us denote them by $\mathbf{G}_s$ and $\mathbf{G}_{s'}$. Now we are ready to state

Lemma": There is a G-map from S to S' if and only if $\mathbf{G}_s \leq \mathbf{G}_{s'}$. In particular, S and S' are equivalent if and only if $\mathbf{G}_s = \mathbf{G}_{s'}$.

Up to equivalence, simple G-sets are characterized by their conjugacy classes of stabilizers. Hence there are at most as many of them as there are conjugacy classes of subgroups of G. In reverse, for any such conjugacy class $|H$ there is a simple G-set S such that $\mathbf{G}_s = |H$. So we end up with a one-to-one correspondence between equivalence classes of simple G-sets and conjugacy classes of subgroups of G.

A simple G-set with stabilizer class $|H$ is readily constructed as follows. For any subgroup $H \in |H$, take S to be G/H, the collection of left cosets gH, and let G act by translation, that is, $g' \in G$ takes gH into $g'gH$. This action is transitive, and H is the stabilizer of the coset $s = H$, so $\mathbf{G}_s = |H$. Two such coset spaces G/H and G/K afford equivalent (transitive) permutation representations if and only if H and K are conjugates. Thus, up to equivalence, simple G-sets are coset spaces, and whenever convenient, we can easily switch back and forth between arbitrary simple G-sets and coset spaces as follows. Let S be a simple G-set and $H \leq G$ be the stabilizer of $s \in S$. Then $gs \leftrightarrow gH$ provides a G-map between S and G/H.

So some differences in comparison with linear representation theory begin to show up. While Schur's lemma turned out to be somewhat weaker in the case of permutation representations, and there is of course no such thing like the »orthogonality relations«, we have an easy construction that yields a complete set of irreducibles for any finite group, while there exists nothing the like in the linear case.

Our next task is to mimic character theory. Characters of permutation representations turn out to be functions defined on the subgroups of the group in question instead of the group elements themselves. They are constant on conjugacy classes of subgroups, and they indeed characterize G-sets up to equivalence. Hence we will stick to the name "character", while they are called "marks" by Burnside and "supercharacters" by Knutson.

Definition: Let S be a G-set. The character χ^S of S attributes to any subgroup $H \leq G$ the number of joint fixed points of its elements,

$$\chi^S(H) := |S_H|, \text{ where}$$

$$S_H := \{s \in S \mid hs = s \text{ for any } h \in H\}.$$

Equivalently, $\chi^S(H)$ is the number of elements in S with stabilizers containing H, since

$$S_H = \{s \in S \mid H \leqslant G_s\}. \tag{15}$$

The following properties of characters are obvious.

1a) Characters are invariant under conjugation, that is, $\chi^S(gHg^{-1}) = \chi^S(H)$.

2a) Equivalent G-sets have identical characters.

3) If a G-set S is the union of disjoint G-subsets $T, U, V, \ldots$, then $\chi^S = \chi^T + \chi^U + \chi^V + \ldots$.

Stronger in fact, both the first two statements admit inversion as follows:

1b) If $\chi^S(K) = \chi^S(H)$ for any G-set S, then K and H are conjugates.

2b) G-sets with identical characters are equivalent.

The last result readily follows from the fact that the simple characters (i. e. the characters of simple G-sets) are linearly independent functions on the subgroups of G. Within the vector space of conjugacy-invariant functions they constitute a basis. Hence any compound character has a unique resolution into simple characters. As a consequence, two G-sets S, S' with identical characters have the same resolution into simple constituents. By glueing together G-maps between equivalent orbits, S and S' are then demonstrated to be equivalent, in turn.

Unlike in linear representation theory, there are simple explicit expressions for all the simple characters of any finite group G. In fact, its character table is nothing else but a condensed version of the matrix that records the structure of the subgroup lattice of G — which would be a square matrix with the subgroups of G as row and column labels, and with (H, K)-entry zero or one, depending on whether H is a subgroup of K or not.

So let us turn to simple characters now. Coset spaces G/K are simple G-sets, and, up to equivalence, any simple G-set is of this type. Since gKg^{-1} is the stabilizer of a coset gK, eq. (15) is readily applied:

$$\begin{aligned} \chi^{G/K}(H) &= \text{no. of cosets } gK \text{ such that } H \leqslant gKg^{-1}, \\ &= \frac{1}{|K|} \text{ no. of } g \in G \text{ such that } H \leqslant gKg^{-1}, \qquad (16) \\ &= \frac{|G|}{|K|} \frac{[H \leqslant |K]}{[|K]}, \end{aligned}$$

where $[H \leq |K]$ and $[|K]$ denote the number of conjugates of K containing H, and the total number of conjugates, respectively. Now let τ be a transversal of the conjugacy classes of subgroups of G, that is, a collection of subgroups, one from each conjugacy class. Then $\{X^{G/K} \mid K \in \tau\}$ is the complete set of simple characters of G, and the square array of numbers

$$M_{HK} := \chi^{G/K}(H); \qquad H, K \in \tau \qquad (17)$$

constitutes the (super) character table of G, Burnside's table of marks of the group in question.

Example 2: For our favourite group D_3 again, we compute its (super) character table. Later we are going to apply it to resolve the permutation representation from the previous example into simple constituents.

$G = D_3 = \{e, c_3, c_3^2, c_2, c_2', c_2''\}$ has altogether six subgroups (including the trivial ones): D_3, $C_3 = \{e, c_3, c_3^2\}$, $C_2 = \{e, c_2\}$, $C_2' = \{e, c_2'\}$, $C_2'' = \{e, c_2''\}$, and $E = \{e\}$.

They fall into four conjugacy classes: $|D_3 = \{D_3\}$, $\mathbf{C}_3 = \{C_3\}$, $\mathbf{C}_2 = \{C_2, C_2', C_2''\}$, $|E = \{E\}$.

The figure below and the table present the subgroup lattice of D_3 and its character table, where the columns make up the simple characters (while the irreducible characters of linear representations are usually tabulated row-wise).

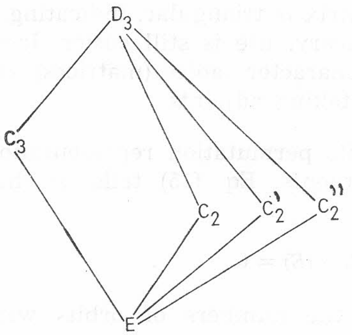

Figure 2

TABLE I

	D_3	C_3	C_2	E
D_3	1	0	0	0
C_3	1	2	0	0
C_2	1	0	1	0
E	1	2	3	6

$$M_{D_3K} = \frac{|D_3|}{|K|} \; \frac{[D_3 \leqslant IK]}{[IK]} = \frac{6}{6} \; \frac{1}{1} \text{ for } K = D_3, \; 0 \text{ otherwise}$$

$$M_{C_3K} = \frac{|D_3|}{|K|} \; \frac{[C_3 \leqslant IK]}{[IK]} = \frac{6}{6} \; \frac{1}{1} \text{ for } K = D_3, \; \frac{6}{3} \; \frac{1}{1} \text{ for } K = C_3, \; 0 \text{ ow.}$$

$$M_{C_2K} = \frac{|D_3|}{|K|} \; \frac{[C_2 \leqslant IK]}{[IK]} = \frac{6}{6} \; \frac{1}{1} \text{ for } K = D_3, \; \frac{6}{2} \; \frac{1}{3} \text{ for } K = C_2, \; 0 \text{ ow.}$$

$$M_{EK} = \frac{|D_3|}{|K|} \; \frac{[E \leqslant IK]}{[IK]} = \frac{|D_3|}{|K|} \text{ for any } K \leqslant D_3$$

In the previous example, the character table turned out to be (lower) triangular; moreover all its diagonal elements were nonzero. These properties hold in general, provided that the subgroups in τ are ordered according to their cardinalities as we did above: $|D_3| = 6 \geq |C_3| = 3 \geq |C_2| = 2 \geq |E| = 1$. In fact, this is evident from the expression

$$M_{HK} = \frac{|G|}{|K|} \; \frac{[H \leqslant IK]}{[IK]}, \tag{18}$$

since $[H \leq |K]$ must be zero for $|H| > |K|$ as well as for $|H| = |K|$ but $|H \neq |K$; and $[H \leq |H] = 1$, so $M_{HH} \neq 0$. Square triangular matrices with non-zero diagonals are ivertible. Equivalently, their colums (as well as their rows) are linearly independent. These facts establish the linear independence of simple characters, and they simultaneously indicate how to resolve a compound character into its (unique) simple components. Let S be a composite G-set with n_K orbits of the type G/K (i. e. with stabilizers in $|K$). Accordingly

$$\chi^S = \sum_{K \in \tau} n_K \chi^{G/K}, \qquad \text{that is,}$$

$$\chi^S(H) = \sum_{K \in \tau} M_{HK} n_K \qquad \text{for any } H \in \tau. \tag{19}$$

Eq. (19) constitutes a system of linear equations for the multiplicities n_K, where the matrix of coefficients is non-singular. Hence it admits a unique solution by matrix inversion. In our case the matrix is triangular, indicating a recursive procedure. In linear representation theory, life is still easier. Irreducible characters are orthonormal, hence the character tables (matrices) are unitary, that is, their inverses are obtained by taking adjoints.

Example 3: For $G = D_3$ again, we resolve its permutation representation from the first example into its simple constituents. Eq. (15) tells us that $\chi(H) =$ no. of sites with symmetry $\geq H$, so

$$\chi(D_3) = 1,\ \chi(C_3) = 3,\ \chi(C_2) = 2,\ \chi(E) = 6.$$

Hence the multiplicities n_H of G/H, that is, the numbers of orbits with stabilizers in $|H$, obey the system of equations

$$\begin{bmatrix} 1 \\ 3 \\ 2 \\ 6 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 2 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 2 & 3 & 6 \end{bmatrix} \begin{bmatrix} n_{D_3} \\ n_{C_3} \\ n_{C_2} \\ n_E \end{bmatrix}$$

which is readily solved, resulting in

$$n_{D_3} = 1,\ n_{C_3} = 1,\ n_{C_2} = 1,\ n_E = 0.$$

Indeed, three is one orbit $\{6\}$ of sites with symmetry $|D_3$, another orbit $\{4, 5\}$ of $\mathbf{C}_3$-symmetric sites, and the sites in the third orbit $\{1, 2, 3\}$ have symmetry $\mathbf{C}_2$.

Though simple in principle, the computation of a (super) character table can be quite a formidable task in practice, since it requires complete survey of the subgroup lattice of the group in question. A computer program that will perform this job for arbitrary finite groups is currently developed by Kerber[7]. For particular types of subgroups there are other expressions for the values of simple characters that are more easily evaluated than formula (16). So e. g. if $H = \langle h \rangle$ is a cyclic subgroup, generated by an element $h \in G$, then $gHg^{-1} \leq K \Longleftrightarrow ghg^{-1} \in K$, which immediately leads to

$$\chi^{G/K}(H) = \frac{|G|}{|H|} \frac{|C_h \cap K|}{|C_h|}. \tag{20}$$

Here $C_h = \{h' = ghg^{-1} \mid g \in G\}$ is the conjugacy class of G containing h. (20) is in fact the character of the linear representation of G induced from the identity representation of K, evaluated at $h \in G$. This is a hint towards connections between linear and permutation representations that we do not follow here, however. Another useful interpretation of characters results from the fact that there are as many G-maps φ: $S' \to S$ between two simple G-sets as there are elements $s \in S$ that are fixed by the stabilizer $G_{s'}$ of an arbitrary element $s' \in S'$. This is in fact true for composite S as well. With the choice of $S' = G/H$, the number of G-maps from G/H to S equals the number of joint fixed points in S of the $h \in H$. This number is just the character of S, evaluated at $H \leq G$. So we end up with

$$\chi^{S}(H) = \text{no. of } G\text{-maps } G/H \to S. \tag{21}$$

Let us close this paragraph with a couple of remarks concerning the analogues of certain constructions from linear representation theory such as subduced/ /induced representations and tensor products. By restricting the action to a subgroup H of G, and G-set S is turned into an H-set, that we will denote by $S \downarrow H$. Clearly this permutation representation of H is the analogue of the linear representation of a subgroup subduced from that of a group. It is enough to consider simple G-sets S, since composite ones may be decomposed into simple G-sets first which then are restricted to H and decomposed in turn. The resolution of restrictions to subgroups of simple G-sets has an algebraic analogue[8] in terms of double cosets: If S is a simple G-set, the H-orbits of S (i. e. the simple constituents of $S \downarrow H$) are in one-to-one correspondence with the double cosets HgG_s in G, where G_s is the stabilizer of an arbitrary element $s \in S$. In terms of coset spaces, we may state more precisely

$$G = \bigcup_{g \in T} HgK \Longleftrightarrow (G/K) \downarrow H \cong \bigcup_{g \in T} H/H \cap gKg^{-1}, \tag{22}$$

Here T is a transversal (system of representatives) of the (H, K)-double cosets in G.

Unlike in linear representation theory, induced permutation representations do not give rise to any appealing problems. Simple H-sets induce simple G-sets in a trivial manner: $H/K \uparrow G \cong G/K$.

Finally, the analogue of the tensor product of G-vectorspaces — associated with what is often called the direct product of representations and the Kronecker product of matrices — is related to double cosets as well. Again we may restrict ourselves to simple G-sets, say S and U. Letting G operate on pairs (s, u) by separately transforming their components, $g\colon (s, u) \longmapsto (gs, gu)$, the cartesian product $S \times U$ is turned into a G-set, and we ask for its resolution into simple constituents. It turns out[8] that they are in one-to-one--correspondence with the double cosets $G_s g G_u$ in G, where G_s and G_u are the stabilizers of arbitrary elements $s \in S$, $u \in U$. In terms of cotes spaces again, we may state

$$G = \bigcup_{g \in T} HgK \Longleftrightarrow (G/H) \times (G/K) \cong \bigcup_{g \in T} G/H \cap gKg^{-1}. \tag{23}$$

The isomorphisms expressed by (22) and (23) clarify the interrelation between the current two, seemingly disjoint, approaches to the enumeration of isomers and isomerizations: the method of generating functions à la Polya and the double coset formalism, as established e. g. in[2,9,10] and,[11–13] respectively.

The table below presents a kind of dictionary, referring to the vocabulary of linear and permutation representations; moreover a few basic results are contrasted.

vector space	—	finite set
linear transformation	—	permutation
linear representation	—	permutation representation
representation space	—	G-set
invariant subspace	—	G-subset
irreducible representation	—	simple G-set, transitivity
irred. inv. subspace	—	orbit

direct sum	— disjoint union
equivalence	— equivalence
Schur's lemma	— weak analogue
orthogonality relations	— no analogue
no analogue	— simple G-sets are coset spaces
character	— mark, supercharacter
conjugacy class of group elements	— conjugacy class of subgroups
character theory	— full analogue, except for orthogonality
subduced representation	— full analogue
induced representation	— trivial analogue
tensor product	— cartesian product.

3. SPECIFIC PROBLEMS AND APPLICATIONS

As mentioned in the introduction, many familiar objects throughout mathematics and sciences are conveniently described in terms of orbits of an appropriate group acting on an appropriate set, in particular of a group acting on a set of mappings by acting on their domain and, possibly, on their range as well. These actions may be traced back to the products of G-sets, discussed at the end of the preceding paragraph, as follows.

Let $P = \{1, 2, \ldots, i, \ldots\}$ and $L = \{A, B, \ldots, X, \ldots\}$ be finite sets. Any mapping φ from P to L can be identified with a subset of the cartesian product set $P \times L$, its graph $\{(i, \varphi(i)) \mid i \in P\}$. Now let a group G act on both, P and L. Then G acts on $P \times L$, as before, by $g \in G$ taking any pair $(i, X) \in P \times L$ into the pair of images (gi, gX). Analogously, $g \in G$ takes any collection of pairs into the collection of image pairs. Hence, the graph of a mapping $\varphi, \{(i, \varphi(i))\}$ is transformed into another subset of $P \times L$, $\{(gi, g\varphi(i))\}$, which is in fact the graph of another mapping φ'. So we have

$$(**) \qquad g : \varphi \to \varphi' \qquad \begin{array}{ll} \text{where} & \varphi'(gi) = g\varphi(i), \text{ or} \\ \text{equivalently} & \varphi'(i) = g\varphi(g^{-1} i), \end{array}$$

and this defines an action of G on L^P the set of all mappings from P to L. Most applications refer to the particular case where G acts trivially or, more plainly, not at all on L: $gX = X$ for any $g \in G$, $X \in L$. Then the action of G on L^P reduces to

$$(*) \qquad g : \varphi \to \varphi' \qquad \begin{array}{ll} \text{where} & \varphi'(gi) = \varphi(i), \text{ or} \\ \text{equivalently} & \varphi'(i) = \varphi(g^{-1} i). \end{array}$$

As the most prominent example of this type, familiar from chemical applications of Polyas enumeration theory, we have

i) *Derivatives of a Symmetrical Parent Compound*

Here P denumerates the positions where substitution may take place in the parent compound, and L is a collection of ligand types. Mappings from P to L obviously represent distributions of ligands with types in L over the sites of the molecular skeleton in question, if $\varphi(i) = X$ is taken to say that there is an X at site i. Now suppose that the skeleton has a non-trivial symmetry, and denote by R its (proper rotational) symmetry group. In this setting, one readily identifies symmetry-equivalent distributions,, i. e. such that are mutually transformed by proper rotations $r \in R$, to represent the same derivative. Evidently, symmetry operations of the (spatially fixed) skeleton permute the distributions. Moreover both, rotations and permutations multiply alike. So R properly acts on L^P, and the orbits of this action are in one-to-one correspondence with the derivatives of the given parent compound, with ligands restricted to the types in L. Similarly, the orbits of G, the full (rotation/reflection) point-symmetry group of an achiral skeleton, correspond to either achiral derivatives or mirror image pairs of chiral ones.

Depending on the structure of the ligands involved, there are several possibilities of how this group action on distributions looks like in detail. First and foremost, a symmetry operations acts by removing the ligands from their original positions to other sites, that is, by permuting the positions of the ligands: $g \in G$ takes to site gi whatever $X \in L$ originally was at site i. If the ligands are sufficiently symmetric, this rearrangement will be the only effect. So we have $g: (i, X) \mapsto (gi, X)$, that is, an action of type (*). Otherwise it may happen that a symmetry operation, besides moving the ligands, also permutes their types. Improper rotations and reflections e. g. take any chiral ligand into its mirror image — independently of its position. So $g \in G$ takes to site gi whatever $X \in L$ originally was at site i, while simultaneously transforming it into gX, $g: (i, X) \mapsto (gi, gX)$, which is an action of type (**). Finally, the fate of a ligand may depend on its position, as would be the case if some ligand type had to be considered a chiral one at certain sites and an achiral one at others. Ref.[14] presents a detailed mathematical discussion of this type of group action, based on the notion of wreath products of permutation groups.

Another important example, perhaps, a bit less familiar within the present context, is provided by the

ii) *Graphs with a Given Number of Vertices*

Here P is the collection of (unordered) pairs $\{i, j\}$ of vertices $i \neq j \in V$, and $L = \{0, 1\}$. Mappings from P to L are readily interpreted as labeled graphs, if $\varphi(\{i, j\}) = 0/1$ is taken to say there isn't/is an edge, connecting the vertices i and j. Now two such labeled graphs φ, φ' are isomorphic if and only if there is a one-to-one correspondence $i \leftrightarrow i'$ between their vertices such that $\varphi(\{i, j\}) = \varphi'(\{i', j'\})$, that is, if and only if they are mutually transformed by a vertex permutation $\pi \in \mathrm{Sym}(V)$ according to $\varphi(\{i, j\}) = \varphi'(\{\pi(i), \pi(j)\})$. Thus there is a type (*)-action of the symmetric group $\mathrm{Sym}(V)$ on L^P, and the orbits of this action correspond to the different unlabeled graphs on $v = |V|$ vertices, that is, to the isomorphism classes of labeled graphs.

This approach to describing graphs admits numerous variations. Replacing e. g. unordered pairs by ordered ones leads to directed graphs, with or without loops, depending on whether the diagonal pairs (i, i) are included. Multigraphs allow for multiple edges, hence they are obtained by enlarging the range to $L = \{0, 1, 2, \ldots\}$. As a final example, graphs with coloured vertices correspond to the orbits of appropriate Young-subgroups of Sym (V): the direct products of symmetric groups, living on the subsets of identically coloured vertices in question. A comprehensive discussion of this line of description can be found in[15]. The monograph[3] by Harary and Palmer presents an impressive survey of the state of the art in the field of enumerating graphs of various types, based on the description in terms of orbits of mappings and the artistry of the generating function method.

Despite their far-reaching similarity, both the theories of permutation representations and of linear representations give rise to distinct characteristic problems, due to their different fields of application, and of course due to the different spaces wherein their objects live: finite sets versus finite-dimensional vector spaces. As far as chemistry is concerned, the theory of groups acting as finite sets apparently has its main applications in the description of molecular structure. So suppose that, quite in general, we have come up with a description in terms of orbits for the objects in some class of our interest. That is, we have established a one-to-one correspondence between the elements of an object set O and the orbits of a group G, acting on a set D of »descriptors«.

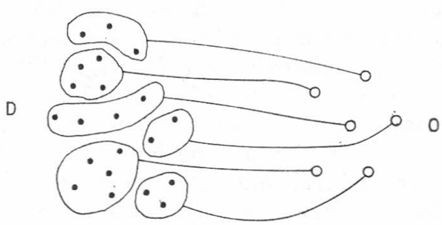

Figure 3

Any such description gives rise to three types of problems.

i) *Enumeration Problems*

As the most obvious application, the number of objects in O is the same as the number of G-orbits in D. So how many orbits are there? This question may be refined by imposing some constraints on the objects which have to be transferable to the descriptors, of course.

ii) *Removal of Redundancy*

Evidently, any such descriptions in terms of orbits is redundant unless all the orbits are singletons. But any transversal, that is, any system of representatives, one from each orbit, provides a redundancy-free description. So how to construct transversals?

iii) *Characterization Problems*

The problem adressed here is that of characterizing the objects by means of invariants, the latter meaning properties of descriptors that are invariant under the group action, that is, they are constant on any orbit. The ultimate goal here is a complete set of invariants which altogether provide distinction of any two orbits — analogous to collections of symptoms (hopefully) characterizing diseases.

So far, almost all applications of permutation group theory in chemistry have been restricted to enumeration problems. The classical problem here is to count isomers*, and the standard solution employs Polya's method or some variation of it. I should like to point out the refined problem of counting isomers of fixed symmetry, comp.[16] and earlier work in the mathematical literature cited there.

Apparently, heterosubstitution of a symmetrical parent compound will in general destroy some of its symmetry elements, thus resulting in a subsymmetry of the parent symmetry. This fact gives rise to a number of questions, referring to a given parent compound, such as

· which subsymmetries can be reached at all by substitution?

·· which is the number of derivatives, with ligands of given types A, B, C, . . ., and with some specified subsymmetry?

··· how many isomers are there, for a given gross formula $A_k B_l C_m \ldots$, and with some specified subsymmetry?

These problems are readily translated into permutation representation theory, starting from the description of derivatives as R-orbits of distributions. The stabilizer R_φ of a distribution φ is its symmetry group, and the conjugacy class of subgroups, $|R_\varphi$, represents the symmetry of the corresponding derivative. Asking for numbers of derivatives with some prescribed symmetry thus amounts to asking for numbers of orbits with stabilizers in some prescribed conjugacy class of subgroups. This is, however, nothing else but the permutation representation analogue of the well-known resolution problem for linear representations, that we discussed at length in the preceding paragraph.

Turning from enumeration problems (which serve as tests as well as rewards for finding good translations of notions from chemistry into mathematics rather than being of relevance in chemistry on their own right) to practical problems, we are immediately faced with the redundancy problem. In view of computer implementation a mathematical description should ideally be meaningful as well as redundancy-free at the same time. Transversals of orbits meet both these conditions. As an example, following the approach of[11] where double cosets were introduced as mathematical analogues of isomers instead of orbits, transversals of double cosets have been employed in algorithmic graph construction[17]. So, given a group action on a finite set, the problem is how to construct a transversal of the orbits. More precisely, the problem is how to perform this in an economical manner, because any straight forward exhaustion method (i. e. selecting a transversal while running through a complete list of elements of the set in question) will always work, of course. This problem is currently under investigation. There is, of course, no general answer to be expected, but some nice results, referring to particular action types, are already available such as the method of stabilizer chains that appears to be due to Sims.[18] It is a mathematical

* In the restricted sense of substitution isomers, that is, of derivatives with the same ligand occurrences.

adaption of the procedure that any chemist would intuitively employ, e. g. in constructing a set of figures, representing the benzene derivatives with some fixed gross formula. Let us e. g. take C_6H_3XYZ. Since all the positions in the benzene ring are equivalent, the X may be taken to be located at site 1, in any derivative. This choice renders 2 and 6 as well as 3 and 5 equivalent; so there are essentially only three different choices for the position of Y, say 2, 3 and 4. In the resulting ortho-pattern, the remaining four positions are mutually inequivalent, thus leaving us with four different choices of where to put Z. The same applies to the intermediate meta--pattern. Finally, in the para-pattern, the pairs 2, 6 and 3, 5 keep being

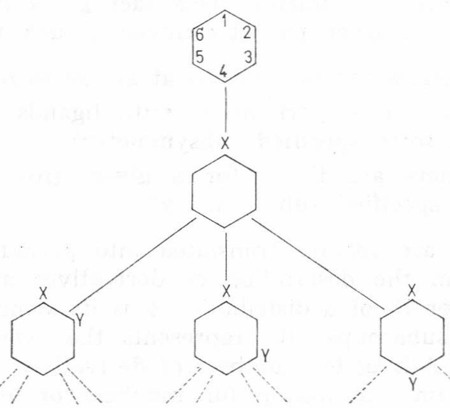

Figure 4

equivalent. So we may select 2 or 3 for the position of Z, thus finishing the list of derivatives.

Turning to iii), the problem of characterizing orbits of mappings by means of invariants appears to be new. A preliminary discussion was given in[19]. Instead of explicating the general scheme — which amounts to refining the gross formula of derivatives to record the »contents« of various orbits of subconfigurations of sites —— we restrict ourselves to the benzene derivatives as an illustrative example, again.

Starting from the familiar three types of double substitution, the idea is to transfer this characterization to multiple substitution by recording, for any (unordered) pair of substituents, how often it occurs as an ortho-pair, as a meta-pair, and as a para-pair, respectively. Thus e. g. the left hand compound below gives rise to the right hand collection of numbers.

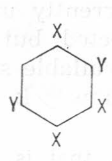

Figure 5

TABLE II

	XX	YY	XY
o	1	0	3
m	1	0	3
p	1	1	0

It turns out that these arrays are enough to distinguish any two isomers. So they provide a complete set of descriptors for benzene derivatives. Now ortho/meta/para label the symmetry types of pairs of positions, that is: the orbits of the dihedral group D_6, acting on the collection of pairs $\{i, j\}$ of sites. The benzene scheme is therefore readily generalized to recording, for $n = 1, 2, \ldots$, the contents of G-orbits of subconfigurations consisting of n sites. These numbers constitute invariants for type (*)-actions. Immediate questions then are whether completeness can be achieved, and for which value of the size n. So e. g. $n = 2$ is enough for benzene derivatives but not for those of (planar) cyclooctatetraene. However $n = 3$, i. e. the contents of triangles, does the job in that particular case, and this appears to be true in general for planar systems, provided that the full point-symmetry is taken into account. So, reaching the end of this paragraph, let us rephrase these observations as follows.

Conjecture: The contents of triangles distinguish any two derivatives of a planar parent compound.

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SAŽETAK

Poziv na permutacijsku reprezentaciju grupa

W. Hässelbarth

Permutacijska reprezentacija grupa odnose se na grupe koje djeluju na konačne skupove permutirajući njihove elemente. Postoji vrlo razvijena teorija permutacijskih reprezentacija, koja je gotovo posve nepoznata izvan matematike. Ovaj rad donosi pregled temeljnih definicija i rezultata i pokazuje perspektivu primjena u »kemijskoj kombinatorici«, gdje ta teorija obećava da će biti od slične upotrebljivosti, kao što je teorija linearnih reprezentacija u kvantnoj kemiji.