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On Lunn-Senior's Mathematical Model of Isomerism in Organic Chemistry. Part I

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ABSTRACT

The aim of this paper is to present a generalization of Lunn-Senior's mathematical model of isomerism in organic chemistry. The main idea of A. C. Lunn and J. K. Senior is that if the type of isomerism is fixed, a molecule with a fixed skeleton and d univalent substituents has a symmetry group $W \leq S_d$ which is generally not the molecule's 3-dimensional symmetry group. The unit character of W induces a representation of the symmetric group S_d which governs the combinatorics of the isomers of the given molecule. Lunn-Senior's thesis is that certain non-negative integers established by this representation are upper boundaries of the corresponding numbers, yielded by the experiment (and often coincide with them). Moreover, the authors define (in a particular case) a partial order among the objects of the model, such that some simple substitution reactions correspond to inequalities. These two groups of data determine the group W, and produce so called "type properties" of the molecule (properties which do not depend on the nature of the univalent substituents). Our hypothesis is that if we replace the unit character of W by any one-dimensional character of W (thus we count only a part of the isomers – those having a maximum property), we also get a type property of the molecule. An instance of that is the inventory of the stereoisomers called chiral pairs. The formalism can be generalized naturally and produces some preliminary chemical results. Especially the partial order is defined and studied in the general case and indicates the possible genetic relations among the corresponding molecules. An important result of E. Ruch which connects the dominance order among partitions and the existence of chiral pairs is obtained as a consequence of a much more general statement. Ruch's formulae for the number of isomers corresponding to a given partition of d are generalized.

1. INTRODUCTION

In this introduction we summarize both the Lunn-Senior's mathematical model from [3], and the content of the present paper.

1.1. Let *AR* be a set of atoms and radicals we are interesting in. The structural (connectivity) formula of a given chemical molecule is usually drawn as an *AR*-labelled graph Γ, where the labels of the vertices of Γ represent atoms or radicals from *AR*, and its (possibly multiple) edges represent valences, or, equivalently, the connectivity data. We note that repetitions of labels are allowed. In the sequel, we identify the graph Γ with the corresponding structural formula. Following [3, I, p. 1030], we use the terms "structure" and "connectivity" as synonyms in order to underline their independence of the 3-dimensional space's limitations.
The mathematical model of Lunn and Senior, which is considered in [3], is based on fixing a certain subset $U(\Gamma)$ of the set $v(\Gamma)$ of vertices of Γ, which has the property that each vertex in $U(\Gamma)$ is an endpoint of exactly one edge of Γ. The labels of the vertices from $U(\Gamma)$ are called *univalent substituents* of Γ. The subgraph $\Sigma(\Gamma)$ of Γ, with set of vertices $v(\Gamma)\backslash U(\Gamma)$ and all edges that connect these vertices, is said to be the *skeleton* of Γ.
Obviously, the division of a structural formula into skeleton and univalent substituents is not unique, but once fixed, this division produces certain properties of the molecule, which, after Lunn and Senior (see [3, I, p. 1031]), are called *type properties*.
Given the skeleton $\Sigma = \Sigma(\Gamma)$, the "degrees of freedom" of the system are constituted by the various ways of distributing the univalent substituents among the unsatisfied valences of the skeleton. Let d be the number of univalent substituents of Γ. We assign to each vertex of the skeleton with unsatisfied valence a number from $1, 2, \ldots, d$, so that different vertices have different numbers, and denote the set of these numbers by $[1, d]$. There are as many different *AR*-labelled graphs Γ with a fixed skeleton Σ, as maps $i\colon [1,d] \to AR$, $k \mapsto i_k$. Thus, the Cartesian product $(AR)^d$ classifies the variety of all structural formulae Γ with a given skeleton Σ. The combinatorial analysis of these Γ's is governed by the representation theory of the symmetric group S_d of the set $[1, d]$.
The fact that the univalent substituents consist of "groups of like individuals", and that "...the differences between them become qualitative, like the differences between red, blue, and yellow geometrical points" (see [3, I, p. 1031]), can be encoded in the mathematical model via dissecting the set $[1, d]$ into several disjoint subsets A_k: $[1, d] = \cup_k A_k$. The group S_d acts naturally on the set Δ_d of all ordered dissections $A = (A_1, A_2, \ldots, A_d)$ of the set $[1, d]$ by virtue of the rule

$$\zeta A = (\zeta(A_1), \zeta(A_2), \ldots, \zeta(A_d)). \tag{1.1.1}$$

Thus, we establish a monomial representation of the symmetric group S_d. We consider the subset T_d of Δ_d, consisting of all ordered dissections A whose components are ordered from largest to smallest. Clearly the elements of the latter can be identified as tabloids with d nodes (see [2, Ch. 2, 2.2.16]). Since S_d is d-transitive on the set $[1, d]$, there exists a one-one correspondence between the orbit space $S_d\backslash T_d$ and the set P_d of all partitions $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_d)$ of the positive integer d. This correspondence can be obtained by factoring out the surjective map $\varphi\colon T_d \to P_d$, $(A_1, A_2, \ldots, A_d) \mapsto (\lambda_1, \lambda_2, \ldots, \lambda_d)$, where λ_k is the cardinality of the set A_k. The S_d-orbit T_λ corresponding to the partition $\lambda \in P_d$ consists of all tabloids of shape λ.
Once a skeleton Σ with d unsatisfied valences is fixed, any tabloid $A \in T_d$ can be considered as structural substituents' *pre-formula* of the d univalent substituents. In other words, A is a pattern of maps which assigns to each number in the component A_1 of that tabloid λ_1 identical univalent substituents x_1 of type 1, to each number in

the component A_2 — λ_2 identical univalent substituents x_2 of type 2, etc., regardless of the nature of these substituents. Moreover, there is a one-one correspondence between the structural substituents' pre-formulae and the structural pre-formulae obtained after joining the skeleton. Then the monomial

$$x_1^{\lambda_1} x_2^{\lambda_2} \dots x_d^{\lambda_d}, \tag{1.1.2}$$

where λ is a partition of d, represents the empirical substituents' pre-formula common to all structural substituents' pre-formulae from the the set T_λ.

Throughout the rest of the paper, in any particular consideration the skeleton will be fixed, so we shall use the expression "structural (respectively, empirical) pre-formula" for structural (respectively, empirical) substituents' pre-formula, and shall identify this structural pre-formula with the corresponding tabloid.

Introducing tabloids, we avoid their equivalent but complicated set theoretic interpretations used in [3, II–]. In particular, our approach allows us to generalize for any partition λ of d the adjacency relations from [3, VI], explicitly defined by Lunn and Senior only for the case $\lambda_1 + \lambda_2 = d$.

1.2. A simple substitution reaction

$$x_1^{\mu_1} \dots x_i^{\mu_i} \dots x_j^{\mu_j} \dots \longrightarrow x_1^{\lambda_1} \dots x_i^{\lambda_i} \dots x_j^{\lambda_j} \dots, \tag{1.2.1}$$

where $\lambda, \mu \in P_d$, and $\mu_1 = \lambda_1, \dots, \mu_i = \lambda_i + 1, \dots, \mu_j = \lambda_j - 1, \dots, \mu_d = \lambda_d$, is reflected by the mathematical model via introducing on the sets P_d and T_d the so called simple raising operators $\rho_{i,j}$, and $R_{i,s}$, respectively (see Sections 2, 3). The operator $R_{i,s}$ acts on a particular structural pre-formula $A = (A_1, A_2, \dots, A_d) \in T_\lambda$ by transferring the element $s \in A_j$ to A_i. This operator mimics the inverse of the operation indicated in the chemical equation (1.2.1): The replacement of one of the univalent substituents x_i of type i in A with an univalent substituent x_j of type j. The structural pre-formula

$$B = (A_1, \dots, A_i \cup \{s\}, \dots, A_j \backslash \{s\}, \dots, A_d) = R_{i,s}A$$

thus obtained is a tabloid of shape μ, and λ and μ are connected via the simple raising operator $\rho_{i,j}$ (see Section 2): $\mu = \rho_{i,j}\lambda$.

A finite product R (respectively, ρ) of simple raising operators $R_{i,s}$ (respectively, $\rho_{i,j}$) is said to be a raising operator. By means of these raising operators, we introduce partial orders on the sets T_d and P_d:

$$A \leq B \text{ if and only if there is a raising operator } R \text{ with } B = RA. \tag{1.2.2}$$

$$\lambda \leq \mu \text{ if and only if there is a raising operator } \rho \text{ with } \mu = \rho\lambda.$$

The latter order is the famous dominance order which plays an important role in the representation theory of the symmetric group (see [2]). We note that in Sections 1 and 3 we state equivalent definitions of the partial orders $A \leq B$, and $\lambda \leq \mu$, respectively, which allow a direct check (in particular, by a computer).

1.3. Now, we turn our attention to the structural pre-formulae as arranged in equivalence classes by certain isomeric relation. In [3], Lunn and Senior consider three isomeric relations:

(a) Univalent substitution isomerism;
(a′) stereoisomerism;
(a″) structural isomerism.
The basic assumption of Lunn and Senior in [3, III] is that for a fixed isomeric relation among (a) – (a″), and for a fixed skeleton Σ, there exists a permutation group $W \leq S_d$, such that the corresponding isomeric classes can be identified with some W-orbits in T_d. More precisely, the group W acts on the set T_d via the rule (1.1.1), and the isomers with skeleton Σ and with d univalent substituents are identified with the elements of the set $T_{d;W} = W\backslash T_d$ of W-orbits in T_d.
The authors emphasize that this group W can be chosen from the large selection of subgroups of S_d, using considerations which have nothing in common with the 3-dimensional space configuration of the respective molecule.
The set T_λ of tabloids of shape λ is a disjoint union of several W-orbits, and if we denote the set of these W-orbits by $T_{\lambda;W}$, we have $T_{d;W} = \cup_{\lambda \in P_d} T_{\lambda;W}$. It should be mentioned that in the set $T_{\lambda;W}$ are gathered all isomers with empirical pre-formula (1.1.2). Let $n_{\lambda;W}$ be the number of elements of the set $T_{\lambda;W}$.

1.4. Let us consider the partial order on $T_{d;W}$ obtained by factoring-out the partial order (1.2.2) in T_d: For $a,\, b \in T_{d;W}$, we write

$$a \leq b \text{ if and only if } A \leq B \text{ for some } A \in a \text{ and } B \in b.$$

This partial order on $T_{d;W}$ is a natural generalization of the adjacency relations considered in [3, VI], so it is a mathematical model of the genetic relations among isomers in organic chemistry.
For any couple λ, and μ of adjacent partitions with $\lambda < \mu$, and $\mu = \rho_{i,j}\lambda$, we consider the subset $R_{\lambda,\mu;W} \subset T_{\lambda;W} \times T_{\mu;W}$, consisting of all ordered pairs (a, b) such that $a < b$, and set $t_{\lambda,\mu;W} = |R_{\lambda,\mu;W}|$.

1.5. Now, we shall enunciate the main statements of Lunn and Senior from [3], summarized in the following

1.5.1. LUNN-SENIOR'S THESIS. *Let Σ be a skeleton with d unsatisfied single valences. One considers molecules with skeleton Σ and substitution's structural pre-formulae which have empirical formula (1.1.2). Then*
1. There exist three permutation groups G, G', $G'' \leq S_d$, such that:
(1a) Any univalent substitution isomer can be identified with a G-orbit in T_d;
(1a′) any stereoisomer can be identified with a G'-orbit in T_d;
(1a″) any structural isomer can be identified with a G''-orbit in T_d.
2. The groups G, G', and $G'' \leq S_d$, are connected in the following way:
(2a) $G = G'$, in case there are no chiral pairs among the univalent substitution isomers, and $G \leq G'$ with $|G' : G| = 2$, in case there are such pairs. In the first case, the G- and G'-orbits coincide and some of them represent the diastereomers. In the last case, each G'-orbit contains either
(2ac) two G-orbits, and the members of any chiral pair are represented by such a couple of G-orbits,
or, coincide with
(2ad) one G-orbit, and any diastereomer is represented by such a G-orbit.
(2b) Any G''-orbit is a disjoint union of G'-orbits.

3. Each simple substitution reaction $b \to a$ of the type (1.2.1) can be identified with the element $(a,b) \in R_{\lambda,\mu;G}$.
4. The terms and relations involved in the statements 1 – 3 do not depend on the nature of the univalent substituents, so they represent type properties of the molecules under consideration.

REMARK 1.5.2. The chemical discourse which has resource to the experiment, and Lunn-Senior's mathematical model, create two languages showing some discrepancy. Below, we state explicitly the chemical definitions of the different types of isomerism described by the mathematical model, in terms of the model itself. Any two compounds in a particular definition are supposed to have the same empirical formula, that is, the corresponding tabloids have the same shape.
Two chemical compounds are said to be ***structural isomers*** if the G''-orbits of their structural formulae are different.
Two chemical compounds are called ***stereoisomers*** if the G'-orbits of their structural pre-formulae are different, but are contained in the same G''-orbit (that is, they have the same connectivity data).
Two chemical compounds are said to be ***univalent substitution isomers*** if the G-orbits of their structural formulae are different.
Two chemical compounds are said to form an ***chiral pair*** if the G-orbits of their structural formulae are different, but are contained in, and cover the same G'-orbit (in particular, they represent the same stereoisomer).
Two chemical compounds are said to be ***diastereomers*** if: (a) the G-orbits O_1 and O_2 of their structural formulae are different; (b) each of O_1 and O_2 coincide with the corresponding G'-orbit; (c) both O_1 and O_2 are contained in the same G''-orbit ((a) - (c) yield that O_1 and O_2 are stereoisomers).

Let $N_{\lambda;\Sigma}$ (respectively, $N'_{\lambda;\Sigma}$, $N''_{\lambda;\Sigma}$) be the number of univalent substitution isomers (respectively, stereoisomers, structural isomers) with fixed skeleton Σ, which have empirical pre-formula (1.1.2). Let $T_{\lambda,\mu;\Sigma}$ be the number of different simple substitution reactions of the type (1.2.1) among the univalent substitution isomers with that skeleton Σ.
According to Lunn-Senior's thesis we have as consequences the following inequalities:

$$N_{\lambda;\Sigma} \le n_{\lambda;G},\ T_{\lambda,\mu;\Sigma} \le t_{\lambda,\mu;G},\ \lambda \in P_d, \tag{1.5.3}$$

$$N'_{\lambda;\Sigma} \le n_{\lambda;G'},\ \lambda \in P_d, \tag{1.5.4}$$

and

$$N''_{\lambda;\Sigma} \le n_{\lambda;G''},\ \lambda \in P_d. \tag{1.5.5}$$

The above inequalities can be used to find the group which corresponds to the particular type of isomerism, as Lunn-Senior's thesis asserts: If one of the inequalities from a row is false for a particular subgroup of the symmetric group S_d, then this subgroup has to be rejected (see [3, IV]). On the other hand, Theorem 5.2.5 shows that the family $(n_{\lambda;W})_\lambda$ of non-negative integers defines both the permutation group $W \le S_d$ up to combinatorial equivalence, and the corresponding induced monomial representation $Ind_W^{S_d}(1_W)$ of the symmetric group S_d — up to isomorphism (here W is one of the groups G, G', or G'').

1.6. A disadvantage of Lunn-Senior's mathematical model is that there are no enough tools immanent to it, in order for two W-orbits to be distinguished.

The aim of this article is to present a mathematical formalism which includes Lunn-Senior's model as a particular case and makes use of the one-dimensional characters of the group W, and the one-dimensional characters of the group $S_\lambda = S_{\lambda_1} \times S_{\lambda_2} \times \cdots \leq S_d$, for picking out of some special W-orbits. A point of departure is the following observation. Let us suppose that there are chiral pairs among the stereoisomers of a given molecule with empirical formula (1.1.2). Then, according to Lunn-Senior's thesis 1.5.1, the group G is a (normal) subgroup of G' with $|G' : G| = 2$. Let $\chi_e : G' \to \{1, -1\}$ be the homomorphism of groups, which assigns 1 to each element of G, and -1 to each element of the complement $G' \backslash G$ of G. Each G'-orbit (which, at least potentially, represents a stereoisomer) coincide with the corresponding G-orbit (and potentially represents a diastereomer), or splits into two G-orbits (thus potentially representing a chiral pair). The G'-orbits O which consist of two G-orbits can be distinguished from the other G'-orbits in the following way. Suppose that $A \in O$ is a tabloid, and let G'_A be the stabilizer of A in G'. We can consider χ_e as a one-dimensional character $\chi_e : G' \to K$, where K is the field of complex numbers. Then O splits into two G-orbits if and only if the character χ_e is identically 1 on the subgroup G'_A. We can count the number of those G'-orbits (let us call them *χ_e-orbits*), using the machinery developed in Section 5. Thus, the one-dimensional character χ_e of the group G' produces a type property of the molecule in question.

On the other hand, it is well known that there is a one-one correspondence between the set $T_{\lambda;W}$ of all W-orbits in T_λ, and the set of all double cosets of S_d modulo (W, S_λ). Let θ be a one-dimensional character of the group S_λ, and let χ be a one-dimensional character of W. We consider the subset $T_{\lambda;\chi,\theta}$ of the set $T_{\lambda;W}$, consisting of all W-orbits which satisfy property (5.1.3), (call them *(χ, θ)-orbits*), and set $n_{\lambda;\chi,\theta} = |T_{\lambda;\chi,\theta}|$.

The hypothesis that for any pair (χ, θ), where W is a group among G, G', and G'', the property (5.1.3) is a type property of the corresponding molecule, recognizable by an experiment, yields the following

1.6.1. EXTENDED LUNN-SENIOR'S THESIS. *Let Σ be a skeleton with d unsatisfied single valences. One considers molecules with skeleton Σ and substitution's structural pre-formulae which have empirical formula (1.1.2). Then*

1. There exist three permutation groups G, G', $G'' \leq S_d$, such that:

(1a) Any univalent substitution isomer can be identified with a G-orbit in T_d;

(1a′) any stereoisomer can be identified with a G'-orbit in T_d;

(1a″) any structural isomer can be identified with a G''-orbit in T_d.

2. The groups G, G', and $G'' \leq S_d$, are connected in the following way:

(2a) $G = G'$, in case there are no chiral pairs among the univalent substitution isomers, and $G \leq G'$ with $|G' : G| = 2$, in case there are such pairs. In the first case, the G and G'-orbits coincide and some of them represent the diastereomers. In the last case, each G'-orbit contains either

(2ac) two G-orbits, and the members of any chiral pair are represented by such a couple of G-orbits,

or, coincide with

(2ad) one G-orbit, and any diastereomer is represented by such a G-orbit.

The χ_e-orbits are those G'-orbits which represent the chiral pairs.

(2b) Any G''-orbit is a disjoint union of G'-orbits.

3. For each sequence $b \to \cdots \to a$ of simple substitution reactions one has $a < b$ and the reaction $b \to a$ can be identified with the inequality $a < b$ in $T_{d;G}$.

4. The terms and relations involved in the statements 1 – 3 do not depend on the nature of the univalent substituents, so they represent type properties of the molecules under consideration.
5. If θ is a one-dimensional character of the group S_λ, and χ is a one-dimensional character of the group W, where W is one of G, G', or G'', then the set of all (χ,θ)-orbits of W in T_λ represents a type property of the molecule.

The isomers which correspond to the hypothetical type property from 1.6.1, item 5, are called (χ,θ)-*isomers*. Let $N_{\lambda;\chi,\theta;\Sigma}$ be the number of all (χ,θ)-isomers with fixed skeleton Σ.
As far as Extended Lunn-Senior's thesis is valid, we have the inequalities

$$N_{\lambda;\chi,\theta;\Sigma} \leq n_{\lambda;\chi,\theta}.$$

1.7. In Section 2 we consider the dominance order on the set M_d consisting of all d-tuples $m = (m_1,\ldots,m_d)$ of non-negative integers whose sum is d, (see [2, Ch. 1, 1.4.6]) and gather the necessary information concerning neighbourhood in M_d and in its subset P_d of all partitions of d.
In Section 3 we introduce tabloids and raising operators which act on their set T_d by analogy with the raising operators from Section 2. Inasmuch as possible, we work in the wider set Δ_d, consisting of all ordered dissections $A = (A_1,\ldots,A_d)$ of the set $[1,d]$. We provide the set Δ_d with a partial order (also called dominance order) such that if we consider the dominance order on the set M_d, then the map $\varphi\colon \Delta_d \to M_d$ from (3.1.1) is a homomorphism of partially ordered sets. The main objective in Section 3 is the study of the equation $\varphi(X) = n$, where $n \in M_d$ (respectively, $n \in P_d$), and the unknown X varies in an interval $[A,B]$ in Δ_d (respectively, in T_d). Theorem 3.4.3 allows us to establish Theorem 3.5.1 which is a criterion for two ordered dissections (tabloids) A and B to be neighbours with respect to the corresponding partial order. This is done by a systematical use of raising operators.
In Section 4 we factor out the constructions from Section 3 with respect to the action of a permutation group $W \leq S_d$, and produce the sets $\Delta_{d;W}$ and $T_{d;W}$, the last one being the sphere of action of the generalized Lunn-Senior's mathematical model of isomerism. Note especially Theorem 4.2.1 which gives necessary and sufficient conditions for two elements a and b to be adjacent in $\Delta_{d;W}$ (respectively, in $T_{d;W}$), as well as Theorem 4.2.3 which is a criterion for a and b to be neighbours there.
Section 5 is devoted to finding explicit expressions for the maximum number of isomers under consideration, according to Lunn-Senior's thesis 1.5.1 and its extension 1.6.1. Here Theorem 5.2.7 is the central result. In Corollary 5.2.10 we give another proof of Ruch's formula which establishes an explicit expression for the numbers $n_{\lambda;W}$ (see [6]). We have to point out Lemma 5.4.3 which shows that when θ is the unit character of the group S_λ, the abstract condition (5.1.3) on the stabilizer W_A of an ordered dissection $A \in a$ is equivalent to to the following maximum property of the W-orbit a:

$$\text{“the } W\text{-orbit } a \text{ consists of } |W : W_\chi| \;\; W_\chi\text{-orbits”},$$

where $W_\chi \leq W$ is the kernel of the one-dimensional character $\chi\colon W \to K$.
Theorem 5.3.1 is a generalization of an important result of E. Ruch which connects the dominance order on the set P_d and the existence of chiral pairs, as it is shown in Subsection 6.2, Theorem 6.2.1. The rest of Section 6 contains illustrations of our approach applied on well known examples: A proof of Kauffmann formulae for the derivatives of naphthalene, and inferences of the genetic relations of ethene and benzene.

2. Partitions

2.1. Let N_d be the set of all d-tuples $m = (m_1, \dots, m_d)$ of integers m_j with $\sum_j m_j = d$. Let M_d be the subset of N_d consisting of all d-tuples m with non-negative components. We denote by P_d the subset of M_d whose elements are all $\lambda = (\lambda_1, \dots, \lambda_d) \in M_d$ with $\lambda_1 \geq \dots \geq \lambda_d$. The elements of P_d are called *partitions of d*. The partition λ can be visualized by the corresponding Young diagram:

$$\lambda = \begin{array}{llllll} \times & \times & \cdots & \cdots & \cdots & \times \\ \times & \times & \cdots & \cdots & \times & \\ & & \vdots & & & \\ \times & \cdots & & & & \end{array} \qquad \begin{array}{c} \lambda_1 \text{ nodes} \\ \lambda_2 \text{ nodes} \\ \vdots \\ \lambda_t \text{ nodes} \end{array} \tag{2.1.1}$$

where λ_t is the last nonzero component of λ. Let $l = (l_1, \dots, l_d)$ and $m = (m_1, \dots, m_d)$ be two elements of the set M_d. In case $l_1 = m_1$, we denote by $q(l, m)$ the maximum number $q \in [1, d]$ such that $l_1 = m_1, \dots, l_q = m_q$. Otherwise, we set $q(l, m) = 0$.
Let $\leq$ be the *dominance order* on N_d (see [4, Ch. I, Sec. 1]). We remind that $l \leq m$ if and only if $\sum_{k=1}^{i} l_k \leq \sum_{k=1}^{i} m_k$ for any $1 \leq i \leq d$. In this case we say that *m dominates l*. It is clear that $\leq$ is a partial order on N_d which induces partial orders on M_d and in P_d, the last two being denoted by the same sign and also named dominance order. Below, the dominance order on P_6 is graphically portrayed.

$$\begin{array}{ccccc} & & (6) & & \\ & & \downarrow & & \\ & & (5,1) & & \\ & & \downarrow & & \\ & & (4,2) & & \\ & \swarrow & & \searrow & \\ (4,1^2) & & & & (3^2) \\ & \searrow & & \swarrow & \\ & & (3,2,1) & & \\ & \swarrow & & \searrow & \\ (3,1^3) & & & & (2^3) \\ & \searrow & & \swarrow & \\ & & (2^2,1^2) & & \\ & & \downarrow & & \\ & & (2,1^4) & & \\ & & \downarrow & & \\ & & (1^6) & & \end{array}$$

Given i, $j \in [1, d]$, we define an operator $\rho_{i,j}\colon N_d \to N_d$ by the formulae

$$\rho_{i,j}(l) = \begin{cases} (l_1, \dots, l_i + 1, \dots, l_j - 1, \dots, l_d) & \text{if } 1 \leq i < j \leq d \\ l & \text{if } 1 \leq j \leq i \leq d. \end{cases}$$

The operators $\rho_{i,j}$ are called *simple raising operators* in N_d. Obviously, any two simple raising operators ρ_{i_1,j_1} and ρ_{i_2,j_2} in N_d commute. Any product $\rho = \rho_{i_1,j_1}\rho_{i_2,j_2}\dots$ of simple raising operators is called *raising operator* in the set N_d. A raising operator is said to be *non-trivial* if it moves at least one element in N_d. Otherwise, it is called *trivial*.

REMARK 2.1.2. We note that the subsets M_d, and P_d of N_d are not closed with respect to the action of a non-trivial raising operator: Given a d-tuple $l \in M_d$, and a simple raising operator $\rho_{i,j}$ with $1 \leq i < j \leq d$, one has $\rho_{i,j}(l) \in M_d$ if and only if $l_j \geq 1$.

If $1 \leq i < j \leq d$, and $\mu = \rho_{i,j}\lambda \in P_d$, then the picture below illustrates the action of the simple raising operator $\rho_{i,j}$ on the Young diagram representing the partition λ:

$$
\lambda = \begin{array}{cccccccccc}
 & \times & \times & \cdots & \cdots & \cdots & \cdots & \cdots & \times & \lambda_1 \text{ nodes} \\
 & \vdots & & & & & & & & \vdots \\
i & \times & \times & \cdots & \cdots & \cdots & \times & & & \lambda_i \text{ nodes} \\
 & \vdots & & & & & \nearrow & & & \vdots \\
j & \times & \times & \cdots & \times & \times & & & & \lambda_j \text{ nodes} \\
 & \vdots & & & & & & & & \vdots \\
 & \times & \cdots & & & & & & & \lambda_t \text{ nodes}
\end{array}
$$

$$\downarrow \quad \rho_{i,j}$$

$$
\mu = \begin{array}{cccccccccc}
 & \times & \times & \cdots & \cdots & \cdots & \cdots & \cdots & \times & \lambda_1 \text{ nodes} \\
 & \vdots & & & & & & & & \vdots \\
i & \times & \times & \cdots & \cdots & \cdots & \times & \times & & \lambda_i + 1 \text{ nodes} \\
 & \vdots & & & & & & & & \vdots \\
j & \times & \times & \cdots & \times & & & & & \lambda_j - 1 \text{ nodes} \\
 & \vdots & & & & & & & & \vdots \\
 & \times & \cdots & & & & & & & \lambda_t \text{ nodes}
\end{array}
$$

2.2. The main aim of the rest of this section is to discuss the conditions under which two elements of M_d (respectively, of P_d) are neighbours with respect to the corresponding partial order.

For any ordered pair (l, m) of elements of N_d we define a sequence of integers

$$r_k = r_k(l, m) = \sum_{i=1}^{k} (m_i - l_i), \quad k = 1, \ldots, d-1,$$

and set $r = r(l, m) = \sum_{k=1}^{d-1} r_k$. It is evident that $l \leq m$ if and only if $r_k(l, m) \geq 0$ for all $k = 1, \ldots, d-1$, and that $r(l, m) = 0$ yields $l = m$.

We borrow part (i) of the next lemma from [4, Ch. I, Sec. 1], and modify it in part (ii).

LEMMA 2.2.1. *(i) If l, $m \in N_d$, then one has $l \leq m$ if and only if there exists a raising operator ρ with $m = \rho(l)$;*

(ii) if $l, m \in M_d$, and if $l < m$, then $m = \rho(l)$ for a raising operator ρ having the following property: There exists a sequence of $r = r(l, m)$ non-trivial simple raising operators $\rho_1, \rho_2, \ldots, \rho_r$ of the type $\rho_{i,i+1}$, $1 \leq i \leq d-1$, such that:

(a) $\rho = \rho_r \cdots \rho_2 \rho_1$;

(b) $\rho_1(l) \in M_d$, $\rho_2\rho_1(l) \in M_d, \ldots, \rho_{r-1} \ldots \rho_2\rho_1(l) \in M_d$;

(c) $l < \rho_1(l) < \rho_2\rho_1(l) < \ldots < \rho_{r-1} \ldots \rho_2\rho_1(l) < m$.

PROOF: (i) Suppose that there exists a raising operator ρ with $m = \rho(l)$. We can assume that $\rho = \rho_{i,j}$, and in this case apparently $l \leq m$. Conversely, let $l \leq m$. Then

$m = \rho(l)$ for

$$\rho = \prod_{k=1}^{d-1} \rho_{k,k+1}^{r_k},$$

where $r_k = r_k(l,m)$;
(ii) We shall prove this statement by induction with respect to $r = r(l,m) \geq 1$. If $r = 1$, then there exists an index $k = i$ such that $r_i = 1$, and $r_k = 0$ for all $k \neq i$, $k = 1, \ldots, d-1$. This implies $m = \rho_{i,i+1}(l)$, and we can set $\rho = \rho_{i,i+1}$. Suppose that part (ii) is true for all $l, m \in M_d$ with $l < m$, and with $r \leq k$, and let $r = k+1$. We set $q = q(l,m)$. Thus, $q < d-1$, and $r_1 = \cdots = r_q = 0$, and $r_{q+1} \geq 1$. Let $\kappa \geq 2$ be the smallest integer with $r_{q+\kappa} = 0$ (integers κ with the property $r_{q+\kappa} = 0$ exist: For instance, $\kappa = d - q$). We have

$$l_{q+2} + \cdots + l_{q+\kappa} \geq l_{q+2} + \cdots + l_{q+\kappa} - m_{q+2} + \cdots + m_{q+\kappa} = r_{q+1} \geq 1.$$

and hence there exists an index j, $q+2 \leq j \leq q+\kappa$, with $l_j \geq 1$. We set $i = q+1$, and $l' = \rho_{i,j}(l)$. Then $l' \in M_d$, $l < l'$, and we have $r_k(l',m) = r_k - 1$ when $k = i, \ldots, j-1$, and $r_k(l',m) = r_k$ otherwise. Since $r_k \geq 1$ for all $k = i, \ldots, q+\kappa-1$, then $r_k(l',m) \geq 0$ for all k, so $l' \leq m$. Moreover, $r(l',m) = r(l,m) - (j-i) = k+1-(j-i) \leq k$, and the inductive assumption yields that there exist $r' = r(l',m)$ simple raising operators $\rho'_1, \ldots, \rho'_{r'}$ of the desired type, such that $m = \rho'(l')$ for $\rho' = \rho'_{r'} \cdots \rho'_1$, and conditions (b) and (c) are satisfied. Taking into account that $\rho_{i,j} = \rho_{i,i+1} \cdots \rho_{j-1,j}$, and that $r = r' + (j-i)$, we get our statement.

THEOREM 2.2.2. *The d-tuples l, m are neighbours in M_d with $l < m$ if and only if there exists $i \in [1,d]$ such that $m = \rho_{i,i+1}(l)$.*

PROOF: Let $m = \rho_{i,i+1}(l)$ and $l \leq n \leq m$. We have $n_k = l_k = m_k$ for $1 \leq k \leq i-1$. Then $l_i \leq n_i \leq m_i = l_i + 1$, so either $n_i = l_i$, or $n_i = m_i$. Further, $l_i + l_{i+1} \leq n_i + n_{i+1} \leq l_i + 1 + l_{i+1} - 1$, hence $l_i + l_{i+1} = n_i + n_{i+1} = m_i + m_{i+1}$. The two cases $n_i = l_i$, or $n_i = m_i$, imply $n = l$, or $n = m$, respectively. Therefore l and m are neighbours with $l < m$.
Now, suppose that the d-tuples l, m are neighbours in M_d with $l < m$. According to Lemma 2.2.1, (ii), we have $m = \rho(l)$, where the raising operator ρ satisfies all conditions (a) - (c). This yields $r = 1$, and hence $m = \rho_{i,i+1}(l)$.

2.3. Here we state [2, Ch. 1, Theorem 1.4.10] which gives necessary and sufficient conditions for two partitions λ, $\mu \in P_d$ to be neighbours in P_d, and refer to the corresponding proof there. It reads as follows:

THEOREM 2.3.1. *The partitions λ, μ are neighbours in P_d with $\lambda < \mu$ if and only if there exist a pair of integers (i,j) with $1 \leq i < j \leq d$, and such that the following two conditions hold:*
(i) One has $\mu = \rho_{i,j}(\lambda)$;
(ii) one has $j = i+1$, or $\lambda_i = \lambda_j$.

In terms of Young diagrams we move the node from the end of j-th row of λ to the end of its i-th row and this move is minimal with the property that we do not leave the subset $P_d \subset \Delta_d$. The last minimum property is equivalent to (ii).

3. DOMINANCE AMONG ORDERED DISSECTIONS AND TABLOIDS

3.1. By an *ordered dissection* of the integer-valued interval $[1,d] = \{1,2,\dots,d\}$ we mean a d-tuple $A = (A_1,\dots,A_d)$ of disjoint subsets $A_i \subset [1,d]$ with $\cup_{i=1}^d A_i = [1,d]$. Sometimes, we shall think of an ordered dissection A as an infinite sequence

$$(A_1,\dots,A_d,A_{d+1},\dots),$$

where $A_k = \emptyset$ for $k > d$. We denote by Δ_d the set of all ordered dissections of $[1,d]$, and define the surjective map

$$\varphi\colon \Delta_d \to M_d, \qquad (3.1.1)$$
$$(A_1,\dots,A_d) \to (|A_1|,\dots,|A_d|).$$

3.2. Each ordered dissection $A = (A_1,\dots,A_d)$ of $[1,d]$ with $|A_1| \geq \dots \geq |A_d|$ is called *tabloid*. Let T_d be the subset of Δ_d consisting of all tabloids. Obviously, $T_d = \varphi^{-1}(P_d)$. The tabloid A can be visualized by placing the elements of A_k in the k-th row of the Young diagram (2.1.1) corresponding to the partition $\lambda = \varphi(A)$ without taking into account their order, for $k = 1,\dots,t$. The next figure illustrates both the tabloid A and the map φ:

$$A = \begin{matrix} a_{1,1}, & a_{1,2}, & \cdots & \cdots & \cdots & a_{1,\lambda_1} & \quad\text{the component } A_1 \\ a_{2,1}, & a_{2,2}, & \cdots & \cdots & a_{2,\lambda_2} & & \quad\text{the component } A_2 \\ & & \vdots & & & & \vdots \\ a_{t,1}, & \cdots & & & & & \quad\text{the component } A_t \end{matrix}$$

$$\downarrow \quad \varphi$$

$$\lambda = \begin{matrix} \times & \times & \cdots & \cdots & \cdots & \times & \quad\lambda_1 \text{ nodes} \\ \times & \times & \cdots & \cdots & \times & & \quad\lambda_2 \text{ nodes} \\ & & \vdots & & & & \vdots \\ \times & \cdots & & & & & \quad\lambda_t \text{ nodes} \end{matrix}$$

We define a partial order on Δ_d via the rule

$$A \leq B \textit{ if and only if } \cup_{k=1}^i A_k \subset \cup_{k=1}^i B_k, \textit{ for any } 1 \leq i \leq d,$$

and call it *dominance order*. In case $A \leq B$ we say that B *dominates* A.
For each $s \in [1,d]$ and each $A \in \Delta_d$ there exists a unique $j \in [1,d]$, such that $s \in A_j$. We set $\varepsilon_A(s) = j$. Thus, any $A \in \Delta_d$ produces a map $\varepsilon_A\colon [1,d] \to [1,d]$.
We introduce a partial order on the set of all maps $[1,d] \to [1,d]$ by virtue of the rule: $\alpha \leq \beta$ if and only if $\alpha(s) \leq \beta(s)$ for all $s \in [1,d]$.
For any two integers $1 \leq i,\ s \leq d$, we define an operator $R_{i,s}\colon \Delta_d \to \Delta_d$ by the formulae

$$R_{i,s}(A) = \begin{cases} (A_1,\dots,A_i \cup \{s\},\dots,A_{\varepsilon_A(s)}\backslash\{s\},\dots,A_d) & \textit{if } \varepsilon_A(s) > i \\ A & \textit{if } \varepsilon_A(s) \leq i. \end{cases}$$

The operators $R_{i,s}$ are said to be *simple raising operators* in Δ_d. Any product $R = R_{i_1,s_1}R_{i_2,s_2}\dots$ of simple raising operators is called *raising operator* on the set Δ_d.
The action of the simple raising operator $R_{i,s}$ on the tabloid A with $B = R_{i,s}A \in T_d$ can be illustrated by the picture below:

$$A = \begin{array}{lllllllll|l}
a_{1,1}, & * & \ldots & * & \ldots & * & * & a_{1,\lambda_1} & & \text{the component } A_1 \\
\vdots & & & & & & & & & \vdots \\
a_{i,1}, & * & \ldots & * & \ldots & a_{i,\lambda_i} & & & & \text{the component } A_i \\
\vdots & & & & & \nearrow & & & & \vdots \\
a_{j,1}, & * & \ldots & * & s & & & & & \text{the component } A_j \\
\vdots & & & & & & & & & \vdots \\
a_{t,1}, & \ldots & & & & & & & & \text{the component } A_t
\end{array}$$

$$\downarrow \quad R_{i,s}$$

$$B = \begin{array}{lllllllll|l}
a_{1,1}, & * & \ldots & * & \ldots & * & * & a_{1,\lambda_1} & & \text{the component } B_1 \\
\vdots & & & & & & & & & \vdots \\
a_{i,1}, & * & \ldots & * & \ldots & a_{i,\lambda_i}, & s & & & \text{the component } B_i \\
\vdots & & & & & & & & & \vdots \\
a_{j,1}, & * & \ldots & * & & & & & & \text{the component } B_j \\
\vdots & & & & & & & & & \vdots \\
a_{t,1}, & \ldots & & & & & & & & \text{the component } B_t
\end{array}$$

It is easy to see that any two simple raising operators commute. Thus, for any $i \in [1,d]$, and for any subset $X \subset [1,d]$ we can define without ambiguity $R_{i,X} = \prod_{x \in X} R_{i,x}$.
For any $i \in [1,d]$, and for any finite family $J = (j_x)_{x \in X}$ of elements of $[1,d]$, we define a raising operator in N_d by $\rho_{i,J} = \prod_{x \in X} \rho_{i,j_x}$.

LEMMA 3.2.1. *(i) For any $A \in \Delta_d$ and any raising operator $R = R_{i_1,s_1} R_{i_2,s_2} \ldots$ one has the inequality $\varepsilon_{R(A)} \leq \varepsilon_A$. If there exists a pair i_k, s_k with $\varepsilon_A(s_k) > i_k$, then $\varepsilon_{R(A)} < \varepsilon_A$;*
(ii) for any subset $X \subset [1,d]$, one has $\varphi(R_{i,X}A) = \rho_{i,\varepsilon_A(X)}\varphi(A)$;
(iii) the map $\varphi\colon \Delta_d \to M_d$ is a homomorphism of partially ordered sets: $\varphi(A) \leq \varphi(B)$ for $A \leq B$; if $A \leq B$ and $\varphi(A) = \varphi(B)$, then $A = B$.

PROOF: (i) It is enough to prove the first statement for $R = R_{i,s}$. When $\varepsilon_A(s) \leq i$, it is obvious. Now, let $\varepsilon_A(s) > i$; Since $i = \varepsilon_{R(A)}(s)$ and since $\varepsilon_A(t) = \varepsilon_{R(A)}(t)$ for $t \neq s$, then $\varepsilon_{R(A)} < \varepsilon_A$, and we have proved both the first statement and the second statement for $R = R_{i,s}$.
For the second statement, we write $R = R' R_{i_k,s_k}$. Then $R(A) = R' R_{i_k,s_k}(A)$ and $\varepsilon_{R(A)} \leq \varepsilon_{R_{i_k,s_k}(A)} < \varepsilon_A$.
(ii) We shall use induction with respect to the number of elements in the set X. When $|X| = 1$, this is trivial. Suppose $|X| \geq 2$, and set $X' = X \backslash \{s\}$, where $s \in X$. $B = R_{i,X'}A$, and $j = \varepsilon_B(s)$. We have

$$\varphi(R_{i,X}A) = \varphi(R_{i,s}R_{i,X'}A) = \varphi(R_{i,s}B) = \rho_{i,j}\varphi(B) =$$

$$\rho_{i,j}\varphi(R_{i,X'}A) = \rho_{i,j}\rho_{i,\varepsilon_A(X')}\varphi(A).$$

Since $s \notin X'$, then $j = \varepsilon_B(s) = \varepsilon_A(s)$, so part (ii) is proved.
(iii) This is a direct consequence of the definitions of the partial orders on Δ_d and M_d.

LEMMA 3.2.2. *Let $A \in \Delta_d$. If $R = R_{i_1,s_1} R_{i_2,s_2} \ldots$ is a raising operator, then $A \leq R(A)$. In particular, if there exists a pair i_k, s_k with $\varepsilon_A(s_k) > i_k$, then $A < R(A)$.*

PROOF: Let $B = R(A)$. We can suppose that $R = R_{i,s}$ and in this case the inequality $A \leq R(A)$ is obvious. Now, Lemma 3.2.1, (i), yields the statement.

3.3. Let $A, B \in \Delta_d$ with $A \leq B$, and let $l = \varphi(A)$ and $m = \varphi(B)$. According to Lemma 3.2.1, (iii), the map φ, defined via (3.1.1), is a homomorphism of partially ordered sets. In particular, φ maps the interval $[A, B]$ into the interval $[l, m]$. In the next two lemmas we begin the study of the equation $\varphi(X) = n$, where $X \in [A, B]$, for various $n \in [l, m]$.

LEMMA 3.3.1. *Let $A, B \in \Delta_d$ with $A \leq B$, and let $l = \varphi(A)$ and $m = \varphi(B)$. Suppose $l \leq n \leq m$, where $n \in M_d$. If for some i, $1 \leq i \leq d$, one has*

$$i - 1 = q(l, n),$$

then there exists a raising operator $R_{i,X}$ with $X \subset A_{i+1} \cup \ldots \cup A_d$, such that $A' = R_{i,X}(A)$ and $l' = \varphi(A')$ satisfy the conditions $A < A' \leq B$, and $l < l' \leq n$, and

$$i \leq q(l', n).$$

PROOF: If $i = d$, then $n = l$, and we choose X to be the empty set. Now, let $i < d$. The equality $i - 1 = q(l, n)$ implies $l_1 = n_1, \ldots, l_{i-1} = n_{i-1}$ and $l_i < n_i$. Hence,

$$l_1 + \cdots + l_i < n_1 + \cdots + n_i \leq m_1 + \cdots + m_i.$$

We choose a subset $X \subset B_1 \cup \ldots \cup B_i \backslash A_1 \cup \ldots \cup A_i$ consisting of $n_i - l_i$ elements. Obviously, $X \subset A_{i+1} \cup \ldots \cup A_d$. We set $A' = R_{i,X}(A)$. Then $l' = \rho_{i,\varepsilon_A(X)}(l)$, and the conditions of the lemma are satisfied.

LEMMA 3.3.2. *Let $A, B \in \Delta_d$ with $A < B$, and let $l = \varphi(A) \in M_d$ and $m = \varphi(B)$. Suppose that $m = \rho_{i,j} l$, where $1 \leq i < j \leq d$, and that there exist an integer $r \geq 1$, and two sequences $(i_k)_{k=1}^r$ and $(s_\kappa)_{\kappa=1}^r$ in the interval $[1, d]$, such that*

$$i = i_1 < i_2 < \ldots < i_r < j, \text{ and } \varepsilon_A(s_\kappa) = i_{\kappa+1}, \text{ for all } 1 \leq \kappa \leq r - 1, \text{ and } \varepsilon_A(s_r) > i_r,$$

and that the components of the ordered dissections $R_{i_1,s_1} \ldots R_{i_r,s_r} A$ and B coincide for all indices in the closed interval $[1, i_r]$. Then there exist two integers i_{r+1}, s_{r+1} in $[1, d]$, such that $i_r < i_{r+1} \leq j$, and $\varepsilon_A(s_{r+1}) = i_{r+1}$, and in case $i_{r+1} < j$ the components of the ordered dissections $R_{i_1,s_1} \ldots R_{i_{r+1},s_{r+1}} A$ and B coincide for all indices in the closed interval $[1, i_{r+1}]$, or one has $B = R_{i_1,s_1} \ldots R_{i_r,s_r} A$ in case $i_{r+1} = j$.

PROOF: It is obvious that the elements $s_1, \ldots, s_r \in [1, d]$ are pairwise different. The condition yields $B_{i_k} = (A_{i_k} \backslash \{s_{k-1}\}) \cup \{s_k\}$ for all $2 \leq k \leq r$, and $B_{i_1} = A_{i_1} \cup \{s_1\}$, and $B_k = A_k$ for all $1 \leq k \leq i_r$ with $k \notin \{i_1, \ldots, i_r\}$.
We shall prove the following

SUBLEMMA. *(i) One has $A_k = B_k$ for all $k \in [i_r + 1, \min\{\varepsilon_A(s_r), j\} - 1]$;*
(ii) one has $\varepsilon_A(s_r) \leq j$.

PROOF: When $\min\{\varepsilon_A(s_r), j\} = i_r + 1$, that is, the interval $[i_r + 1, \min\{\varepsilon_A(s_r), j\} - 1]$ is empty, the statement is trivial. Let $\min\{\varepsilon_A(s_r), j\} > i_r + 1$. We have

$$A_{i_1} \cup \ldots \cup A_{i_r} \cup A_{i_r+1} \subset B_{i_1} \cup \ldots \cup B_{i_r} \cup B_{i_r+1}.$$

Since

$$B_{i_1} \cup \ldots \cup B_{i_r} = A_{i_1} \cup \ldots \cup A_{i_r} \cup \{s_r\},$$

and since $s_r \notin A_{i_r+1}$, we obtain $A_{i_r+1} \subset B_{i_r+1}$. Then $l_{i_r+1} = m_{i_r+1}$ implies $A_{i_r+1} = B_{i_r+1}$. Suppose that

$$A_{i_r+1} = B_{i_r+1}, \ldots, A_{k-1} = B_{k-1},$$

for $i_r + 1 < k \leq \min\{\varepsilon_A(s_r), j\} - 1$. Then we get $A_k \subset B_k \cup \{s_r\}$, and because of $s_r \notin A_k$, we obtain $A_k \subset B_k$. Then $l_k = m_k$ implies $A_k = B_k$. Thus, part (i) is proved by induction.
(ii) Suppose the opposite, that is, $\varepsilon_A(s_r) > j$. Then, according to part (i), we have $A_j \subset B_j \cup \{s_r\}$. Again $s_r \notin A_j$ yields $A_j \subset B_j$. On the other hand, $l_j - 1 = m_j$, which is a contradiction.

We set $i_{r+1} = \varepsilon_A(s_r)$. According to the above Sublemma, $i_r < i_{r+1} \leq j$ and $A_k = B_k$ for all $i_r < k < i_{r+1}$. Thus, we have $A_{i_{r+1}} \subset B_{i_{r+1}} \cup \{s_r\}$, so $A_{i_{r+1}} \backslash \{s_r\} \subset B_{i_{r+1}}$.
Case 1. $i_{r+1} < j$.
Since $l_{i_{r+1}} = m_{i_{r+1}}$, there exists an element $s_{r+1} \in B_{i_{r+1}}$ such that $s_{r+1} \notin A_{i_{r+1}} \backslash \{s_r\}$, and $B_{i_{r+1}} = (A_{i_{r+1}} \backslash \{s_r\}) \cup \{s_{r+1}\}$. Since $s_k \in B_{i_k}$, we have $s_{r+1} \neq s_k$ for $1 \leq k \leq r$. This implies $s_{r+1} \notin A_{i_{r+1}}$; hence $\varepsilon_A(s_{r+1}) > i_{r+1}$. Having this information, it is not hard to check that the components of the ordered dissections B and $R_{i_1,s_1} \ldots R_{i_r,s_r} R_{i_{r+1},s_{r+1}} A$ coincide for all indices in the closed interval $[1, i_{r+1}]$.
Case 2. $i_{r+1} = j$.
Since $l_j - 1 = m_j$, then $A_j \backslash \{s_r\} = B_j$, so the components of the ordered dissections $R_{i_1,s_1} \ldots R_{i_r,s_r} A$ and B coincide for all indices in the closed interval $[1, j]$. Now, we shall prove that $B_k = A_k$ for all $j+1 \leq k \leq d$. We have $\cup_{k=1}^{j} A_k = \cup_{k=1}^{j} B_k$, so $A_{j+1} \subset B_{j+1}$. Therefore the equality $l_{j+1} = m_{j+1}$ gives $A_{j+1} = B_{j+1}$. Obvious induction finishes the proof.

3.4. We say that $l \in M_d$ and $m \in M_d$ are *adjacent* with $l < m$ if $m = \rho_{i,j} l$ for some pair of integers (i, j) with $1 \leq i < j \leq d$. Given A, $B \in \Delta_d$, we set $l = \varphi(A)$ and $m = \varphi(B)$. The ordered dissections A and B are called *adjacent* with $A < B$ if $A < B$, and l and m are adjacent (with $l < m$). According to Lemma 3.2.1, (ii), if the ordered dissections A and B satisfy $B = R_{i,s} A$ for some pair $i, s \in [1, d]$ such that $\varepsilon_A(s) > i$, then A and B are adjacent in Δ_d with $A < B$. The converse statement is not true. The situation is clarified in the next theorem.

THEOREM 3.4.1. *Let $A, B \in \Delta_d$ be adjacent with $A < B$, and let $l = \varphi(A) \in M_d$ and $m = \varphi(B)$. Suppose that $m = \rho_{i,j} l$, where $1 \leq i < j \leq d$. Then there exist an integer $r \geq 1$, and two sequences $(i_k)_{k=1}^{r+1}$ and $(s_\kappa)_{\kappa=1}^{r}$ in the interval $[1, d]$, such that*

$$i = i_1 < i_2 < \ldots < i_{r+1} = j, \text{ and } \varepsilon_A(s_\kappa) = i_{\kappa+1} \text{ for all } 1 \leq \kappa \leq r.$$

and that $B = R_{i_1,s_1} \ldots R_{i_r,s_r} A$.

PROOF: We apply several times Lemma 3.3.2. In order to begin, we note that $q(l, m) = i - 1$, and use Lemma 3.3.1 in case $n = m$, thereby producing the first pair (i_1, s_1) with $i_1 = i$, and $\varepsilon_A(s_1) > i$. It is obvious that the components of the ordered dissections B and $R_{i_1,s_1} A$ coincide for all indices in the interval $[1, i_1]$.

THEOREM 3.4.2. *Let $A, B \in \Delta_d$ with $A \leq B$, and let $l = \varphi(A) \in M_d$ and $m = \varphi(B) \in M_d$. For any $n \in M_d$ with $l \leq n \leq m$, and $q(l,n) = q$, there exists a raising operator of the type $R = R_{d,X_d} \dots R_{q+1,X_{q+1}}$ with $X_k \subset A_{k+1} \cup \dots \cup A_d$, such that $A' = R(A)$ satisfies the conditions $A \leq A' \leq B$, and $\varphi(A') = n$.*

PROOF: We shall use induction with respect to $q = q(l,n)$. If $q = d$, then $l = n$ and the ordered dissection $A' = R(A) = A$ for the trivial operator $R = R_{d,X_d} R_{d+1,X_{d+1}}$, $X_d = X_{d+1} = \emptyset$, works. Suppose that if $i \leq q \leq d$, then there exists a raising operator of the type $R = R_{d,X_d} \dots R_{q+1,X_{q+1}}$, such that $A' = R(A)$ satisfies the conditions $A \leq A' \leq B$, and $\varphi(A') = n$. If $q = i - 1$, then Lemma 3.3.1 yields the existence of a raising operator of the type $R'' = R_{i,X_i}$ with $X_i \subset A_{i+1} \cup \dots \cup A_d$, such that $A'' = R''(A)$, and $l'' = \rho_{i,\varepsilon_A(X_i)}(l)$, satisfy the conditions $l < l'' \leq n$, and $i \leq q(l'', n) \leq d$, and $A < A'' \leq B$, and $\varphi(A'') = l''$. Hence, there exists a raising operator

$$R' = R_{d,X_d} \dots R_{i+1,X_{i+1}},$$

such that $A' = R'(A'')$ satisfies the conditions $A'' < A' \leq B$, and $\varphi(A') = n$. Since $A' = R(A)$ for

$$R = R'R'' = R_{d,X_d} \dots R_{i+1,X_{i+1}} R_{i,X_i} = R_{d,X_d} \dots R_{q+1,X_{q+1}},$$

the induction is done.

THEOREM 3.4.3. *(i) Let $A, B \in \Delta_d$ with $A < B$. Let $l = \varphi(A)$ and $m = \varphi(B)$. Then the restriction φ_1 of the map φ on the interval $[A, B]$ in Δ_d is a surjection*

$$\varphi_1 \colon [A, B] \to [l, m],$$

and one has $\varphi_1^{-1}((l,m)) = (A, B)$;
(ii) let $A, B \in T_d$ with $A \leq B$. Let $\lambda = \varphi(A)$ and $\mu = \varphi(B)$. Then the restriction φ_2 of the map φ on the interval $[A, B]$ in T_d is a surjection

$$\varphi_2 \colon [A, B] \to [\lambda, \mu],$$

and one has $\varphi_2^{-1}((\lambda, \mu)) = (A, B)$;

PROOF: (i) The surjectivity of φ_1 is a consequence of Theorem 3.4.2. The inclusion $\varphi_1^{-1}((l,m)) \subset (A, B)$ is obvious. Suppose that $A < C < B$. Then the assumption that $\varphi(C) = l$, or $\varphi(C) = m$ leads to a contradiction with Lemma 3.2.1, (iii).
(ii) If $C \in M_d$ with $\varphi(C) \in P_d$, then $C \in T_d$, so part (i) assures that the map φ_2 is surjective. The rest of the proof is identical to that of part (i).

THEOREM 3.4.4. *If $A, B \in \Delta_d$ then $A \leq B$ if and only if there exists a raising operator R such that $B = R(A)$.*

PROOF: The "if" part follows from Lemma 3.2.2. Now, let $A, B \in \Delta_d$, $A \leq B$, with $l = \varphi(A)$ and $m = \varphi(B)$. In case $A = B$ we choose R to be the trivial operator. Now, let $A < B$. We apply Theorem 3.4.2 in the particular case $n = m$ to produce a raising operator R such that the ordered dissection $A' = R(A)$ satisfies $A \leq A' \leq B$, and $\varphi(A') = m = \varphi(B)$. Then Lemma 3.2.1, (iii), yields that $B = A' = R(A)$.

3.5. Here we find necessary and sufficient conditions for two ordered dissections, or for two tabloids to be neighbours with respect to the partial orders on Δ_d and on T_d, respectively.

THEOREM 3.5.1. *(i) The ordered dissections $A, B \in \Delta_d$ are neighbours in Δ_d with $A < B$, if and only if there exist $i \in [1, d]$ and $s \in [1, d]$, such that $\varepsilon_A(s) = i + 1$ and $B = R_{i,s}(A)$;*
(ii) the tabloids $A, B \in T_d$ are neighbours in T_d with $A < B$, if and only if there exist a pair of integers (i, j) with $1 \le i < j \le d$, an integer $r \ge 1$, and two sequences $(i_k)_{k=1}^{r+1}$ and $(s_\kappa)_{\kappa=1}^{r}$ in the interval $[1, d]$, such that:

$$j = i + 1 \text{ or } |A_i| = |A_j|, \tag{3.5.2}$$

and

$$i = i_1 < i_2 < \ldots < i_{r+1} = j, \text{ and } \varepsilon_A(s_\kappa) = i_{\kappa+1}, \text{ for all } 1 \le \kappa \le r, \tag{3.5.3}$$

and that

$$B = R_{i_1,s_1} \ldots R_{i_r,s_r} A. \tag{3.5.4}$$

PROOF: (i) We set $l = \varphi(A)$, and $m = \varphi(B)$. Suppose that the pair $A, B \in \Delta_d$ is such that $B = R_{i,s}(A)$ with $\varepsilon_A(s) = i + 1$. Then Lemma 3.2.1, (ii), yields $m = \rho_{i,i+1} l$. Hence, according to Theorem 2.2.2 we have that l and m are neighbours with $l < m$, and now Theorem 3.4.3, (i), yields that A and B are neighbours in Δ_d with $A < B$.

Assume that $A, B \in \Delta_d$ are neighbours in Δ_d with $A < B$. Theorem 3.4.3, (i), implies that l and m are neighbours in M_d with $l < m$. Then, due to Theorem 2.2.2 there exist an integer $1 \le i < d$, such that $m = \rho_{i,i+1} l$, and Theorem 3.4.1 yields the existence of an element $s \in [1, d]$ with $\varepsilon_A(s) = i + 1$ and $B = R_{i,s} A$.

(ii) Suppose that $A, B \in T_d$ are neighbours in T_d with $A < B$. Denote $\lambda = \varphi(A)$ and $\mu = \varphi(B)$. Theorem 3.4.3, (ii), implies that the partitions λ and μ are neighbours in P_d with $\lambda < \mu$. Due to Theorem 2.3.1, there is a pair of integers (i, j) with $1 \le i < j \le d$, and such that $\mu = \rho_{i,j} \lambda$. Therefore, according to Theorem 3.4.1, there exist an integer $r \ge 1$, and two sequences $(i_k)_{k=1}^{r+1}$ and $(s_\kappa)_{\kappa=1}^{r}$ in the interval $[1, d]$, such that (3.5.3) and (3.5.4) hold. Moreover, Theorem 2.3.1 yields (3.5.2).

Conversely, suppose that the conditions (3.5.2) – (3.5.4) are satisfied. Applying the map φ on the equality (3.5.4), we obtain

$$\mu = \varphi(B) = \rho_{i_1,i_2} \cdots \rho_{i_r,i_{r+1}} \varphi(A) = \rho_{i,j} \lambda.$$

Therefore Theorem 2.3.1 assures that the partitions λ and μ are neighbours in P_d with $\lambda < \mu$. Now, according to Theorem 3.4.3, (ii), the tabloids A and B are neighbours in T_d with $A < B$.

The next picture illustrates Theorem 3.5.1, (ii), case $j > i + 1$, when there exists a sequence of "virtual substitutions" which starting with A produces B. Here "virtual" means that during the intermediate steps we leave the set T_d of tabloids.

$$A = \begin{array}{lllllllllll|l}
 & a_{1,1}, & a_{1,2}, & * & * & \dots & * & * & * & a_{1,\lambda_1} & & A_1 \\
 & \vdots & & & & & & & & & & \vdots \\
i = i_1 & a_{i,1}, & a_{i,2}, & * & * & \dots & * & a_{i,\lambda_i} & & & & A_i \\
 & \vdots & & & & & & & & & & \vdots \\
i_r & * & * & * & * & \dots & * & * & & & & A_{i_r} \\
 & \vdots & & \nwarrow & & & & & & & & \\
j = i_{r+1} & a_{j,1}, & * & * & s_r, & \dots & * & a_{j,\lambda_j} & & & & A_j \\
 & \vdots & & & & & & & & & & \vdots \\
 & a_{t,1}, & \dots & & & & & & & & & A_t
\end{array}$$

$$\downarrow R_{i_r,s_r}$$

$$\begin{array}{lllllllllll|l}
 & a_{1,1}, & a_{1,2}, & * & * & \dots & * & * & * & a_{1,\lambda_1} & & A_1 \\
 & \vdots & & & & & & & & & & \vdots \\
i = i_1 & a_{i,1}, & a_{i,2}, & * & * & \dots & * & a_{i,\lambda_i} & & & & A_i \\
 & \vdots & & & & & & & & & & \vdots \\
i_{r-1} & * & * & * & * & \dots & * & * & & & & A_{i_{r-1}} \\
 & \vdots & & & \nearrow & & & & & & & \vdots \\
i_r & * & s_r, & s_{r-1}, & * & \dots & * & * & * & & & A_{i_r} \cup \{s_r\} \\
 & \vdots & & & & & & & & & & \\
j = i_{r+1} & a_{j,1}, & * & * & \hat{s}_r, & \dots & a_{j,\lambda_j} & & & & & A_j \setminus \{s_r\} \\
 & \vdots & & & & & & & & & & \vdots \\
 & a_{t,1}, & \dots & & & & & & & & & A_t
\end{array}$$

$$\downarrow \quad R_{i_{r-1},s_{r-1}}$$

$$\vdots$$

$$\downarrow$$

$$B = \begin{array}{lllllllllll|l}
 & a_{1,1}, & a_{1,2}, & * & * & \dots & * & * & * & a_{1,\lambda_1} & & A_1 \\
 & \vdots & & & & & & & & & & \vdots \\
i = i_1 & a_{i,1}, & a_{i,2}, & * & * & \dots & * & a_{i,\lambda_i}, & s_1 & & & A_i \cup \{s_1\} \\
 & \vdots & & & & & & & & & & \vdots \\
j = i_{r+1} & a_{j,1}, & * & * & \hat{s}_r, & \dots & a_{j,\lambda_j} & & & & & A_j \setminus \{s_r\} \\
 & \vdots & & & & & & & & & & \vdots \\
 & a_{t,1}, & \dots & & & & & & & & & A_t
\end{array}$$

(The hat over a number stands for absence of that number.)

4. The model

4.1. The symmetric group S_d acts on the set Δ_d of all ordered dissections of $[1, d]$ by the rule (1.1.1). Let $W \leq S_d$ be a subgroup of the symmetric group S_d. Then the group W acts on the set Δ_d via the same rule. We denote by $\Delta_{d;W}$ the factor-set $W \backslash \Delta_d$

and by $T_{d;W}$ — the factor-set $W\backslash T_d$. Let $\psi_W: \Delta_d \to \Delta_{d;W}$ be the natural surjection. For any $A \in \Delta_d$ we denote by $O_W(A)$ its W-orbit in Δ_d, so $\psi_W(A) = O_W(A)$. Since $\varphi(\sigma A) = \varphi(A)$ for any $A \in \Delta_d$ and for any $\sigma \in W$, the map φ factors out to a map $\varphi_W: \Delta_{d;W} \to M_d$.

LEMMA 4.1.1. *If A, $B \in \Delta_d$ are neighbours in Δ_d with $A < B$ and if $\zeta A \leq B$, then $\zeta A < B$, and the ordered dissections ζA and B are neighbours in Δ_d.*

PROOF: The equalities $\zeta A = B$, $\varphi(\zeta A) = \varphi(B)$, together with Lemma 3.2.1, (iii), yield $A = B$ which is a contradiction. Hence $\zeta A < B$. According to Theorem 3.5.1, (i), the fact that A and B are neighbours implies $B = R_{i,s}A$ for some $i \in [1,d]$ and $s \in [1,d]$ with $\varepsilon_A(s) = i+1$. Then, using Lemma 3.2.1, (ii), we obtain $\varphi(B) = \varphi(R_{i,s}A) = \rho_{i,i+1}(\varphi(A)) = \rho_{i,i+1}(\varphi(\zeta A))$. Now, we apply Lemma 3.3.2 for the pair ζA and B, and get the existence of an integer $s_1 \in [1,d]$ with $\varepsilon_A(s_1) = i+1$, such that $B = R_{i,s_1}(\zeta A)$. The neighbourhood of ζA and B follows from Theorem 3.5.1, (i).

Let a, $b \in \Delta_{d;W}$, and $A \in a$, $B \in b$. We define a partial order $\leq$ on the factor-set $\Delta_{d;W}$ via the rule:

$$a \leq b \text{ if and only if there exists a } \sigma \in W, \text{ such that } \sigma A \leq B.$$

THEOREM 4.1.2. *(i) Let a, $b \in \Delta_{d;W}$, and $A \in a$, $B \in b$ with $A \leq B$. Then the restriction ψ_1 of the map ψ_W on the union of the intervals $[\sigma A, B]$, $\sigma \in W$, in Δ_d, is a surjection*

$$\psi_1: \cup_{\sigma \in W}[\sigma A, B] \to [a,b]$$

onto the interval $[a,b]$ in $\Delta_{d;W}$, and one has $\psi_1^{-1}((a,b)) = \cup_{\sigma\in W}(\sigma A, B)$;
(ii) let a, $b \in T_{d;W}$, and $A \in a$, $B \in b$ with $A \leq B$. Then the restriction ψ_2 of the map ψ_W on the union of the intervals $[\sigma A, B]$, $\sigma \in W$, in T_d, is a surjection

$$\psi_2: \cup_{\sigma \in W}[\sigma A, B] \to [a,b]$$

onto the interval $[a,b]$ in $T_{d;W}$, and one has $\psi_2^{-1}((a,b)) = \cup_{\sigma\in W}(\sigma A, B)$;

PROOF: (i) By definition $a \leq b$. Suppose that $a \leq c \leq b$, where $c \in \Delta_{d;W}$ and let $C \in c$. There exist σ, $\tau \in W$, such that $\sigma A \leq C$ and $\tau C \leq B$. Then $\tau\sigma A \leq \tau C \leq B$ and $\psi_1(\tau C) = c$, so the surjectivity of the map ψ_1 is proved. Assume that $\sigma A < C < B$, for some $\sigma \in W$, and some $C \in \Delta_d$. By definition, $a \leq c \leq b$, where $c = \psi_1(C)$. If $a = c$, or $c = b$, then $\tau C < C$, or $\tau B < B$, respectively, for an appropriate $\tau \in W$, which contradicts to Lemma 3.2.1, (iii). Therefore $\cup_{\sigma\in W}(\sigma A, B) \subset \psi_1^{-1}((a,b))$, and part (i) holds.
(ii) We note that $c \in T_{d;W}$, and $C \in c$, where $C \in \Delta_d$, yield $C \in T_d$. Thus, the proof of part (i) holds in this case, too.

4.2. It is said that $a, b \in \Delta_{d;W}$ are *adjacent* with $a < b$ if there exist $A \in a$, and $B \in b$, which are adjacent with $A < B$ (see 3.4). In other words, there exists a pair of integers (i,j) with $1 \leq i < j \leq d$, and such that $\varphi_W(b) = \rho_{i,j}(\varphi_W(a))$.

THEOREM 4.2.1. *The elements $a, b \in \Delta_{d;W}$ are adjacent with $a < b$, if and only if there exist $A \in a$, and $B \in b$, with $A < B$, and there exist a pair of integers (i,j) with*

$1 \leq i < j \leq d$, *an integer* $r \geq 1$, *and two sequences* $(i_k)_{k=1}^{r+1}$ and $(s_\kappa)_{\kappa=1}^{r}$ *in the interval* $[1, d]$, *such that:*

$$i = i_1 < i_2 < \ldots < i_{r+1} = j, \text{ and } \varepsilon_A(s_\kappa) = i_{\kappa+1}, \text{ for all } 1 \leq \kappa \leq r.$$

and that

$$B = R_{i_1, s_1} \ldots R_{i_r, s_r} A. \tag{4.2.2}$$

PROOF: The necessity holds because of Theorem 3.4.1. For the converse statement we apply the map φ on the equality (4.2.2) and obtain $\varphi(B) = \rho_{i,j}(\varphi(A))$. Hence a and b are adjacent with $a < b$.

THEOREM 4.2.3. *(i) The elements* $a, b \in \Delta_{d;W}$ *are neighbours in* $\Delta_{d;W}$ *with* $a < b$, *if and only if there exist* $A \in a$, *and* $B \in b$, *with* $A < B$, *and there exist* $i \in [1, d]$ *and* $s \in [1, d]$, *such that* $\varepsilon_A(s) = i + 1$ *and* $B = R_{i,s}(A)$;
(ii) the elements $a, b \in T_{d;W}$ *are neighbours in* $T_{d;W}$ *with* $a < b$, *if and only if there exist* $A \in a$, *and* $B \in b$, *with* $A < B$, *and there exist a pair of integers* (i, j) *with* $1 \leq i < j \leq d$, *an integer* $r \geq 1$, *and two sequences* $(i_k)_{k=1}^{r+1}$ *and* $(s_\kappa)_{\kappa=1}^{r}$ *in the interval* $[1, d]$, *such that:*

$$j = i + 1 \text{ or } |A_i| = |A_j|,$$

and

$$i = i_1 < i_2 < \ldots < i_{r+1} = j, \text{ and } \varepsilon_A(s_\kappa) = i_{\kappa+1}, \text{ for all } 1 \leq \kappa \leq r,$$

and that $B = R_{i_1, s_1} \ldots R_{i_r, s_r} A$.

PROOF: Using Lemma 4.1.1, and Theorem 4.1.2, (i) (respectively (ii)), we get that a and b are neighbours in $\Delta_{d;W}$ (respectively, in $T_{d;W}$) with $a < b$ if and only if A and B are neighbours in Δ_d (respectively, in T_d) with $A < B$. Then Theorem 3.5.1. (i) (respectively (ii)), finishes the proof of part (i) (respectively, of part (ii)).

5. COUNTING OF ISOMERS

5.1. The set T_d can be stratified using the fibres $T_\lambda = \varphi^{-1}(\lambda)$ of the map $\varphi: T_d \to P_d$, where λ runs through the set P_d. Clearly, T_λ is the set of all tabloids of shape λ. Since the symmetric group S_d is d-transitive on $[1, d]$, the set of fibres T_λ, $\lambda \in P_d$, coincides with the set $S_d \backslash T_d$ of S_d-orbits in T_d.
The orbit T_λ contains the tabloid I with components $I_1 = [1, \lambda_1], I_2 = [\lambda_1 + 1, \lambda_1 + \lambda_2], \ldots$, and its stabilizer is the subgroup $S_\lambda = S_{\lambda_1} \times \cdots \times S_{\lambda_d} \leq S_d$. Thus

$$S_d / S_\lambda \simeq T_\lambda, \tag{5.1.1}$$

$$vS_\lambda \mapsto vI,$$

is an isomorphism of S_d-sets.
Let us fix a S_d-orbit T_λ and consider the action of the permutation group $W \leq S_d$ on T_λ, which is induced by the action (1.1.1) of S_d. Let us denote by $T_{\lambda;W}$ the orbit space $W \backslash T_\lambda$. Then the isomorphism (5.1.1) of S_d-sets can also be considered as an isomorphism of W-sets, and moreover, it factors out to a bijection

$$W \backslash S_d / S_\lambda \simeq T_{\lambda;W},$$

$$W v S_\lambda \mapsto vI,$$

between the set of double cosets of S_d modulo (W, S_λ), and the set of W-orbits in T_λ.
Let $A = vI \in T_\lambda$. The stabilizer W_A of A in the group W consists of all $\sigma \in W$ such that $v^{-1}\sigma v \in S_\lambda$, or, equivalently, $\sigma \in vS_\lambda v^{-1}$. Hence $W_A = W \cap vS_\lambda v^{-1}$.
We fix a one-dimensional character $\chi: W \to K$ and a one-dimensional character $\theta: S_\lambda \to K$. For a given $v \in S_d$, and $A = vI$, the rule

$$\beta_v: W_A \to K, \tag{5.1.2}$$

$$\beta_v(\sigma) = \chi(\sigma)\theta(v^{-1}\sigma v),$$

defines a one-dimensional character of the stabilizer W_A.
If $B = \tau A$ for some $\tau \in W$, then $B = \tau vI$ and $W_B = \tau W_A \tau^{-1}$. For the corresponding one-dimensional character $\beta_{\tau v}: W_B \to K$, we have

$$\beta_{\tau v}(\tau\sigma\tau^{-1}) = \chi(\tau\sigma\tau^{-1})\theta(v^{-1}\tau^{-1}\tau\sigma\tau^{-1}\tau v) = \beta_v(\sigma),$$

where $\sigma \in W_A$. Therefore, given a W-orbit $a \in T_{\lambda;W}$, the statements

$$\text{“}\beta_v(\sigma) = 1 \text{ for any } \sigma \in W_A\text{”} \tag{5.1.3}$$

are simultaneously true or false regardless of the representative $A = vI \in a$. We denote by $T_{\lambda;\chi,\theta}$ the subset of $T_{\lambda;W}$ consisting of those W-orbits a for which the statement (5.1.3) is true for some representative $A = vI \in a$, and call them (χ, θ)-*orbits* of the group W. In particular, $T_{\lambda;1_W,1_{S_\lambda}} = T_{\lambda;W}$.
In case $\theta = 1_{S_\lambda}$ for all $\lambda \in P_d$, the (χ, θ)-orbits of the group shall be called simply χ-*orbits* of the group W. Thus the χ-orbits are those W-orbits $a \in T_d$ for which there exists a tabloid $A \in a$ such that the character χ is identically 1 on its stabilizer W_A (see (5.1.3)). Then the last condition holds for all tabloids $A \in a$. We set $T_{\lambda;\chi} = T_{\lambda;\chi,1_{S_\lambda}}$, and $T_{d;\chi} = \cup_{\lambda\in P_d} T_{\lambda;\chi}$.
We introduce the following families of non-negative integers: $n_{\lambda;\chi,\theta} = |T_{\lambda;\chi,\theta}|$, $n_{\lambda;\chi} = |T_{\lambda;\chi}|$, and $n_{\lambda;W} = |T_{\lambda;W}|$, where $\lambda \in P_d$. Note that $n_{\lambda;\chi} = n_{\lambda;\chi,1_{S_\lambda}}$, and $n_{\lambda;W} = n_{\lambda;1_W} = n_{\lambda;1_W,1_{S_\lambda}}$.

5.2. Now, our aim is to find an explicit formula for the number $n_{\lambda;\chi,\theta}$ of (χ, θ)-orbits of the group W in the set T_λ, where $\lambda \in P_d$. We shall use freely terminology, notation and results from [4, Ch. I] and [7, Ch. I - II].
For any finite set X we denote by $|X|$ the number of its elements. For a partition $\lambda \in P_d$ we shall use also the notation $(1^{m_1}, 2^{m_2}, \ldots, d^{m_d})$, where m_k is the number of the parts of λ, which are equal to k, $1 \le k \le d$. Given a permutation $\zeta \in S_d$, we denote by $\varrho(\zeta)$, and also, by $(1^{c_1(\zeta)}, 2^{c_2(\zeta)}, \ldots, d^{c_d(\zeta)})$ the corresponding partition of the number d. We set

$$C(W, S_\lambda) = \{(\sigma, \eta) \in W \times S_\lambda \mid \varrho(\sigma) = \varrho(\eta)\}.$$

Let t be the length of the partition λ. Then $S_\lambda = S_{\lambda_1} \times \cdots \times S_{\lambda_t}$, so any $\eta \in S_\lambda$ has the form $\eta = \eta_1 \ldots \eta_t$, where $\eta_k \in S_{\lambda_k}$. Thus $\varrho(\eta) = \varrho(\eta_1) \cup \ldots \cup \varrho(\eta_t)$, where $\varrho(\eta_k) \in P_{\lambda_k}$. The one-dimensional character θ has a unique decomposition $\theta = \theta_1 \ldots \theta_t$, where θ_k is either the signature or the unit character of S_{λ_k}. We set

$$L_\lambda = \{(\alpha, \alpha^{(1)}, \ldots, \alpha^{(t)}) \in P_d \times P_{\lambda_1} \times \cdots \times P_{\lambda_t} \mid \alpha = \alpha^{(1)} \cup \ldots \cup \alpha^{(t)}\},$$

and define a map

$$\gamma_1 : W \times S_{\lambda_1} \times \cdots \times S_{\lambda_t} \to P_d \times P_{\lambda_1} \times \cdots \times P_{\lambda_t},$$

$$(\sigma, \eta_1 \ldots, \eta_t) \mapsto (\varrho(\sigma), \varrho(\eta_1), \ldots, \varrho(\eta_t)).$$

Then $C(W, S_\lambda) = \gamma_1^{-1}(L_\lambda)$. Let $L'(W, S_\lambda) \subset L_\lambda$ be the image of $C(W, S_\lambda)$ via the map γ_1. The restriction of γ_1 on $C(W, S_\lambda)$ is a surjective map

$$\gamma : C(W, S_\lambda) \to L'(W, S_\lambda).$$

If $(\alpha, \alpha^{(1)}, \ldots, \alpha^{(t)}) \in L'(W, S_\lambda)$, then

$$\gamma^{-1}(\alpha, \alpha^{(1)}, \ldots, \alpha^{(t)}) = W_\alpha \times K_{\alpha^{(1)}} \times \cdots \times K_{\alpha^{(t)}}, \tag{5.2.1}$$

where W_α is the subset of the group W, consisting of all permutations of cycle-type α, and $K_{\alpha^{(k)}}$ is the conjugacy class in S_{λ_k}, corresponding to the partition $\alpha^{(k)} \in P_{\lambda_k}$. The set W_α is a union of conjugacy classes of the group W:

$$W_\alpha = C_1^{(\alpha)} \cup \ldots \cup C_{i_\alpha}^{(\alpha)}. \tag{5.2.2}$$

We set

$$L(W, S_\lambda) = L'(W, S_\lambda) \backslash \{((1), (1), \ldots, (1))\}. \tag{5.2.3}$$

Let $h_\lambda = h_{\lambda_1} h_{\lambda_2} \ldots$, where h_{λ_k} is the λ_k-th complete symmetric function (see [4, Ch. I, Sec. 2]).

LEMMA 5.2.4. *Let $W \leq S_d$ be a permutation group and let $\chi : W \to K$ be a one-dimensional character.*
(i) The characteristic of the induced monomial representation $Ind_W^{S_d}(\chi)$ is equal to the generalized cycle index

$$Z(\chi; p_1, \ldots, p_d) = \frac{1}{|W|} \sum_{\sigma \in W} \chi(\sigma) p_1^{c_1(\sigma)} \ldots p_d^{c_d(\sigma)},$$

where $p_s = x_0^s + x_1^s + \cdots$ are the power sums;
(ii) one has $n_{\lambda;\chi,\theta} = \langle Ind_W^{S_d}(\chi), Ind_{S_\lambda}^{S_d}(\theta) \rangle_{S_d}$;
(iii) one has $n_{\lambda;\chi} = \langle Z(\chi; p_1, \ldots, p_d), h_\lambda \rangle$;
(iv) if $Z(\chi; p_1, \ldots, p_d) = \sum_{\lambda \in P_d} a_\lambda m_\lambda$, where m_λ are the monomial symmetric functions, then $a_\lambda = n_{\lambda;\chi}$.

PROOF: (i) Let ψ be the map which assigns to each substitution $\zeta \in S_d$ the symmetric function $p_{\varrho(\zeta)}$ (see [4, Ch. I, Sec. 7]). According to Frobenius reciprocity law,

$$ch(Ind_W^{S_d}(\chi)) = \langle Ind_W^{S_d}(\chi), \psi \rangle_{S_d} =$$

$$\langle \chi, Res_W^{S_d}(\psi) \rangle_W = Z(\chi; p_1, \ldots, p_d).$$

(ii) Using Frobenius reciprocity law and Mackey's theorem (see [7, Ch. II, 7.4, Proposition 15]), we have

$$\langle Ind_W^{S_d}(\chi), Ind_{S_\lambda}^{S_d}(\theta)\rangle_{S_d} = \langle \chi, Res_W^{S_d} Ind_{S_\lambda}^{S_d}(\theta)\rangle_{S_d} =$$
$$\langle \chi, \sum_{v\in\Upsilon} Ind_{W_v}^W(\theta_v)\rangle_W,$$

where Υ is a system of representatives of the double cosets of S_d modulo (W, S_λ), and θ_v is the one-dimensional character of the group $W \cap vS_\lambda v^{-1}$ given by the formula $\theta_v(x) = \theta(v^{-1}xv)$. Further,

$$\langle Ind_W^{S_d}(\chi), Ind_{S_\lambda}^{S_d}(\theta)\rangle_{S_d} = \sum_{v\in\Upsilon} \langle \chi, Ind_{W_v}^W(\theta_v)\rangle_W =$$
$$\sum_{v\in\Upsilon} \langle Res_{W_v}^W(\chi), \theta_v\rangle_{W_v} = |\{v \in \Upsilon \mid Res_{W_v}^W(\chi) = \theta_v\}|.$$

Since $\theta^2 = 1$, then

$$\{v \in \Upsilon \mid Res_{W_v}^W(\chi) = \theta_v\} = \{v \in \Upsilon \mid \beta_v(\sigma) = 1 \text{ for any } \sigma \in W_v\}.$$

Therefore, using the isomorphism (5.1.4) of W-sets we get

$$\langle Ind_W^{S_d}(\chi), Ind_{S_\lambda}^{S_d}(\theta)\rangle_{S_d} = n_{\lambda;\chi,\theta}.$$

(iii) Indeed, the characteristic map ch is an isometric isomorphism of rings (see [4, Ch. I, Sec. 7, 7.3]), so in particular,

$$\langle Ind_W^{S_d}(\chi), Ind_{S_\lambda}^{S_d}(1_{S_\lambda})\rangle_{S_d} = \langle ch(Ind_W^{S_d}(\chi)), ch(Ind_{S_\lambda}^{S_d}(1_{S_\lambda}))\rangle.$$

Evidently, $ch(Ind_{S_\lambda}^{S_d}(1_{S_\lambda})) = h_\lambda$. According to Lemma 5.2.4, (i), we have

$$ch(Ind_W^{S_d}(\chi)) = Z(\chi; p_1, \ldots, p_d).$$

Therefore

$$n_{\lambda;\chi} = n_{\lambda;\chi,1_{S_\lambda}} = \langle Ind_W^{S_d}(\chi), Ind_{S_\lambda}^{S_d}(1_{S_\lambda})\rangle_{S_d} = \langle Z(\chi; p_1, \ldots, p_d), h_\lambda\rangle.$$

(iv) Using part (iii) we obtain

$$n_{\lambda;\chi} = \langle \sum_{\alpha\in P_d} a_\alpha m_\alpha, h_\lambda\rangle = \sum_{\lambda\in P_d} a_\alpha \langle m_\alpha, h_\lambda\rangle = a_\lambda.$$

The last equality holds because of [4, Ch. I, Sec. 4, 4.5].

THEOREM 5.2.5. *Let $W, W' \leq S_d$ be two permutation groups. Then the following four statements are equivalent:*
(i) One has $n_{\lambda;W} = n_{\lambda;W'}$ for all $\lambda \in P_d$;
(ii) one has

$$Z(1_W; p_1, \ldots, p_d) = Z(1_{W'}; p_1, \ldots, p_d);$$

(iii) the induced monomial representations $Ind_W^{S_d}(1_W)$, and $Ind_{W'}^{S_d}(1_{W'})$, of the symmetric group S_d, are equivalent;
(iv) there exists a one-one correspondence between the groups W and W', such that the corresponding permutations have the same type of cycle decomposition.

PROOF: Lemma 5.2.4, (i) and (iv), applied for 1_W, and $1_{W'}$, and [4, Ch. I, Sec. 7, 7.3]) yield the equivalence of (i), (ii), and (iii). It is easily seen that the equality of cycle indices in (ii) is equivalent to (iv).

REMARK 5.2.6. According to [3, IV], two permutation groups W, $W' \leq S_d$ which satisfy (iv) are said to be *literally conformal.* In [5, Ch. I, Sec. 25], it is shown that each of (ii) and (iv) is equivalent to the so called *combinatorial equivalence* of W and W'.

For any partition $\lambda \in P_d$, $\lambda = (1^{m_1}, 2^{m_2}, \ldots, d^{m_d})$, we set

$$z_\lambda = 1^{m_1} m_1! 2^{m_2} m_2! \ldots d^{m_d} m_d!.$$

THEOREM 5.2.7. *Let $W \leq S_d$ be a permutation group and let $\chi : W \to K$ be a one-dimensional character. Let $n_{\lambda;\chi,\theta}$ be the number of all (χ, θ)-orbits of the group W in the set T_λ. Then one has*

$$n_{\lambda;\chi,\theta} = \frac{d!}{|W|\lambda_1! \ldots \lambda_d!} +$$

$$\frac{1}{|W|} \sum_{(\alpha,\alpha^{(1)},\ldots,\alpha^{(t)}) \in L(W,S_\lambda)} (\sum_{i=1}^{i_\alpha} |C_i^{(\alpha)}| \chi(C_i^{(\alpha)})) \frac{z_\alpha}{z_{\alpha^{(1)}} \ldots z_{\alpha^{(t)}}} \theta_1(K_{\alpha^{(1)}}) \ldots \theta_t(K_{\alpha^{(t)}}),$$

where $C_1^{(\alpha)}, \ldots, C_{i_\alpha}^{(\alpha)}$ are the conjugacy classes of W consisting of permutations of cycle-type $\alpha \in P_d$, and $K_{\alpha^{(k)}}$ is the conjugacy class in S_{λ_k}, corresponding to the partition $\alpha^{(k)} \in P_{\lambda_k}$, $k = 1, \ldots t$.

PROOF: The characteristic map ch is an isometry, and Lemma 5.2.4, (i), holds, so

$$\langle Ind_W^{S_d}(\chi), Ind_{S_\lambda}^{S_d}(\theta)\rangle_{S_d} = \langle ch(Ind_W^{S_d}(\chi)), ch(Ind_{S_\lambda}^{S_d}(\theta))\rangle =$$

$$\langle Z(\chi; p_1, \ldots, p_d), Z(\theta; p_1, \ldots, p_d)\rangle = \langle \frac{1}{|W|} \sum_{\sigma \in W} \chi(\sigma) p_{\varrho(\sigma)}, \frac{1}{|S_\lambda|} \sum_{\eta \in S_\lambda} \theta(\eta) p_{\varrho(\eta)}\rangle =$$

$$\frac{1}{|W||S_\lambda|} \sum_{\sigma \in W} \sum_{\eta \in S_\lambda} \chi(\sigma)\theta(\eta) \langle p_{\varrho(\sigma)}, p_{\varrho(\eta)}\rangle.$$

According to [4, Ch. I, Sec. 4, 4.7], we obtain

$$\langle Ind_W^{S_d}(\chi), Ind_{S_\lambda}^{S_d}(\theta)\rangle_{S_d} = \frac{1}{|W||S_\lambda|} \sum_{(\sigma,\eta) \in C(W,S_\lambda)} \chi(\sigma)\theta(\eta) z_{\varrho(\sigma)}. \tag{5.2.8}$$

Further, we use the partition of the set $C(W, S_\lambda)$ into the fibres of the surjective map γ, as well as their representation (5.2.1). Thus, we have

$$\langle Ind_W^{S_d}(\chi), Ind_{S_\lambda}^{S_d}(\theta)\rangle_{S_d} =$$

$$\frac{1}{|W||S_\lambda|} \sum_{(\alpha,\alpha^{(1)},\ldots,\alpha^{(t)}) \in L'(W,S_\lambda)} \sum_{(\sigma,\eta_1,\ldots,\eta_t) \in W_\alpha \times K_{\alpha^{(1)}} \times \cdots \times K_{\alpha^{(t)}}} \chi(\sigma)\theta_1(\eta_1) \ldots \theta_t(\eta_t) z_\alpha =$$

$$\frac{1}{|W|\lambda_1! \ldots \lambda_t!} \sum_{(\alpha,\alpha^{(1)},\ldots,\alpha^{(t)}) \in L'(W,S_\lambda)} (\sum_{i=1}^{i_\alpha} |C_i^{(\alpha)}| \chi(C_i^{(\alpha)})) \prod_{k=1}^{t} \frac{\lambda_k!}{z_{\alpha^{(k)}}} \theta_k(K_{\alpha^{(k)}}) z_\alpha =$$

$$\frac{1}{|W|}\sum_{(\alpha,\alpha^{(1)},\ldots,\alpha^{(t)})\in L'(W,S_\lambda)}\left(\sum_{i=1}^{i_\alpha}|C_i^{(\alpha)}|\chi(C_i^{(\alpha)})\right)\frac{z_\alpha}{z_{\alpha^{(1)}}\ldots z_{\alpha^{(t)}}}\theta_1(K_{\alpha^{(1)}})\ldots\theta_t(K_{\alpha^{(t)}})=$$

$$\frac{d!}{|W|\lambda_1!\ldots\lambda_d!}+$$

$$\frac{1}{|W|}\sum_{(\alpha,\alpha^{(1)},\ldots,\alpha^{(t)})\in L(W,S_\lambda)}\left(\sum_{i=1}^{i_\alpha}|C_i^{(\alpha)}|\chi(C_i^{(\alpha)})\right)\frac{z_\alpha}{z_{\alpha^{(1)}}\ldots z_{\alpha^{(t)}}}\theta_1(K_{\alpha^{(1)}})\ldots\theta_t(K_{\alpha^{(t)}}).$$

In the last two equalities we make use of (5.2.2) and (5.2.3). Now, Lemma 5.2.4, (ii), yields the result.

The specialization $\chi = 1_W$, and $\theta = 1_{S_\lambda}$, in Theorem 5.2.7 entails

COROLLARY 5.2.9. *One has*

$$n_{\lambda;W} = \frac{d!}{|W|\lambda_1!\ldots\lambda_d!}+$$

$$\frac{1}{|W|}\sum_{(\alpha,\alpha^{(1)},\ldots,\alpha^{(t)})\in L(W,S_\lambda)}|W_\alpha|\frac{z_\alpha}{z_{\alpha^{(1)}}\ldots z_{\alpha^{(t)}}}.$$

COROLLARY 5.2.10 (RUCH'S FORMULA). *One has*

$$n_{\lambda;W} = \frac{n!}{|W||S_\lambda|}\sum_{\alpha\in P_d}\frac{|W_\alpha||(S_\lambda)_\alpha|}{|K_\alpha|}.$$

PROOF: Using the equality (5.2.8) for $\chi = 1_W$, and $\theta = 1_{S_\lambda}$, we have

$$n_{\lambda;W} = \frac{1}{|W||S_\lambda|}\sum_{(\sigma,\eta)\in C(W,S_\lambda)} z_{\varrho(\sigma)} =$$

$$\frac{1}{|W||S_\lambda|}\sum_{\alpha\in P_d}\sum_{(\sigma,\eta)\in W\times S_\lambda,\varrho(\sigma)=\varrho(\eta)=\alpha} z_\alpha =$$

$$\frac{1}{|W||S_\lambda|}\sum_{\alpha\in P_d}|W_\alpha||(S_\lambda)_\alpha|z_\alpha =$$

$$\frac{n!}{|W||S_\lambda|}\sum_{\alpha\in P_d}\frac{|W_\alpha||(S_\lambda)_\alpha|}{|K_\alpha|}.$$

REMARK 5.2.11. Let Γ and Δ be two graphs with d vertices, and with automorphism groups W and S_λ, respectively. The number calculated in Theorem 5.2.7 coincides with the number of superpositions of Γ and Δ, such that the one-dimensional character (5.1.2) is identically 1 on their stabilizers (that is, their automorphism groups). The last number can also be obtained by an appropriate generalization of Redfield's superposition theorem (see [1]).

5.3. Here we shall consider the family of non-negative integers $n_{\lambda;\chi} = |T_{\lambda;\chi}|$, $\lambda \in P_d$.

THEOREM 5.3.1. *Let χ be a one-dimensional character χ of the group $W \leq S_d$, and let $\lambda, \mu \in P_d$. If $\lambda \leq \mu$, then $n_{\lambda;\chi} \geq n_{\mu;\chi}$.*

PROOF: According to Lemma 5.2.4, (iii), we have $n_{\lambda;\chi} - n_{\mu;\chi} = \langle Z(\chi; p_1, \dots, p_d), h_\lambda - h_\mu \rangle$. Then [4, Ch. I, Sec. 7, Example 9 (b)] implies that the difference $h_\lambda - h_\mu$ is a non-negative integral linear combination of the Schur functions s_ν, $\nu \in P_d$. On the other hand, $Z(\chi; p_1, \dots, p_d)$ is the characteristic of the induced monomial representation $Ind_W^{S_d}(\chi)$, so it also is a linear combination of s_ν with non-negative integral coefficients. Therefore the above scalar product is non-negative.

The specialization $\chi = 1_W$ yields

COROLLARY 5.3.2. *If $\lambda, \mu \in P_d$, and $\lambda \leq \mu$, then $n_{\lambda;W} \geq n_{\mu;W}$.*

5.4. Below, Lemma 5.4.3 for $I = T_d$ gives a combinatorial interpretation of the set $T_{d;\chi}$ of all χ-orbits. We shall work in a more general setup.
Let W be a finite group which acts on a set I. For each element $i \in I$ we denote by W_i its stabilizer in W. Let χ be a one-dimensional character of the group W with kernel $H \leq W$.

LEMMA 5.4.1. *The following statements hold:*
(i) The inclusion $W_i \leq H$, and the equality $|W_i : H_i| = 1$ are equivalent for any $i \in I$;
(ii) if O is a W-orbit in I, then all H-orbits in O have the same number of elements, and their number is a divisor of the index $|W : H|$.

PROOF: (i) It is enough to note that $H_i = H \cap W_i$.
(ii) Let $i \in O$. Since H is a normal subgroup of W, then $\sigma H_i \sigma^{-1} \leq H$ for all $\sigma \in W$. Therefore $|H : H_{\sigma i}| = |H : \sigma H_i \sigma^{-1}| = |H : H_i|$, that is, each H-orbit in O has the same number of elements. Then using the equality

$$|W : H||H : H_i| = |W : W_i||W_i : H_i|, \tag{5.4.2}$$

where $i \in I$, we obtain immediately that the number of H-orbits in O is a divisor of $|W : H|$.

If O is a W-orbit in I, and if one has $W_i \leq H$ for some $i \in O$ (and, hence, for all $i \in O$), then O is said to be a χ-*orbit*.

LEMMA 5.4.3. *The following two statements are equivalent:*
(i) The W-orbit O is a χ-orbit;
(ii) the W-orbit O contains exactly $|W : H|$ H-orbits;
(iii) the W-orbit O contains maximal number of H-orbits.

PROOF: Let O be a χ-orbit. The equality (5.4.2) and Lemma 5.4.1, (i), yield $|W : H||H : H_i| = |O|$ for $i \in O$. Because of Lemma 5.4.1, (ii), the indices $|H : H_i|$ do not depend on $i \in O$ and all are equal to the number of elements of any H-orbit in O. Therefore (ii) holds. Conversely, suppose that the W-orbit O contains exactly $|W : H|$ H-orbits, and let $i \in O$. Lemma 5.4.1, (ii), implies $|W : W_i| = |O| = |W : H||H : H_i|$. Comparing with (5.4.2), we obtain $|W_i : H_i| = 1$. Due to Lemma 5.4.1, (i), O is a χ-orbit. Finally, Lemma 5.4.1, (ii), yields that part (iii) is equivalent to part (ii).

6. First applications

6.1. Now, we apply Corollary 5.2.9 to obtain Kauffmann formulae for the number of the derivatives of naphthalene, $C_{10}H_8$.
The group of substitution isomerism of naphthalene is the subgroup G of S_8, consisting of the elements

$$(1),(12)(34)(56)(78),(13)(24)(57)(68),(14)(23)(58)(67)$$

(see [3, IX, D]). The unit (1) of G produces the term $\frac{1}{4}\frac{8!}{\lambda_1!\ldots\lambda_8!}$. The other 3 elements of G have cycle structure (2^4), so $|G_{(2^4)}| = 3$.
Suppose that the set $L(G,S_\lambda)$ contains an element $(\alpha,\alpha^{(1)},\ldots,\alpha^{(t)})$ with $\alpha = (2^4)$. Then α is to be the cycle-type of an element of $S_\lambda = S_{\lambda_1}\times\cdots\times S_{\lambda_t} \leq S_8$, where t is the length of the partition λ of 8.
In case at least one of the components λ_k is odd, we establish a contradiction, so in this case

$$n_{\lambda;G} = \frac{1}{4}\frac{8!}{\lambda_1!\ldots\lambda_8!}.$$

In the rest of the cases, all components λ_k are to be even, so $\lambda = (2\mu_1, 2\mu_2, \ldots, 2\mu_t)$, where $\mu = (\mu_1,\mu_2,\ldots,\mu_t)$ is a partition of 4. Now, we have

$$L(W,S_\lambda) = \{((2^4),(2^{\mu_1}),(2^{\mu_2}),\ldots,(2^{\mu_t}))\},$$

and

$$n_{\lambda;G} = \frac{1}{4}\frac{8!}{\lambda_1!\ldots\lambda_8!} + \frac{1}{4}|W_{(2^4)}|\frac{z_{(2^4)}}{z_{(2^{\mu_1})}z_{(2^{\mu_2})}\cdots} =$$

$$\frac{1}{4}\frac{8!}{\lambda_1!\ldots\lambda_8!} + \frac{3}{4}\frac{2^4 4!}{2^{\mu_1}\mu_1!2^{\mu_2}\mu_2!\ldots} =$$

$$\frac{1}{4}\frac{8!}{\lambda_1!\ldots\lambda_8!} + \frac{3}{4}\frac{4!}{(\frac{\lambda_1}{2})!(\frac{\lambda_2}{2})!\ldots}.$$

Thus, we have obtained Kauffmann formulae.

6.2. This subsection is devoted to chiral pairs. Let Σ be a skeleton with d unsatisfied single valences. Suppose that among the substitution derivatives of a given parent substance with skeleton Σ there is an chiral pair. Then according to Lunn-Senior Thesis 1.5.1, (2a), the group $G' \leq S_d$ of stereoisomerism contains the group G of substitution isomerism as a subgroup of index 2. In particular, G is a normal subgroup of G'. Let $\chi_e\colon G' \to K$ be the one-dimensional complex valued character with kernel G. We have $\chi_e(\sigma) = 1$ for $\sigma \in G$ and $\chi_e(\sigma) = -1$ for $\sigma \in G'\backslash G$. Lemma 5.4.1, (ii), for $I = T_d$ and $W = G'$ implies that each G'-orbit O contains either two or one G-orbit. Lunn-Senior Thesis 1.5.1, part (2ae), and part (2ad), makes the corresponding identifications with the chiral pairs, and with the diastereomers, respectively. Lemma 5.4.3 applied for $I = T_d$ and $W = G'$ shows that the set $T_{d;\chi_e}$ of χ_e-orbits contains the chiral pairs. In particular, part (2a) of the Extended Lunn-Senior Thesis 1.6.1 is justified.
Now, as a direct consequence of Theorem 5.3.1 for $W = G'$ and $\chi = \chi_e$, we obtain a result of E. Ruch of special beauty.

THEOREM 6.2.1 (RUCH). *If a distribution of ligands according to the partition μ amounts to a chiral molecule, and λ is dominated by μ , then also a distribution according to λ yields a chiral molecule.*

6.3. Now using our approach we shall present the classical Körner's relations between the di-, and tri-substitution derivatives of benzene C_6H_6. The exposition below follows that of Lunn and Senior.

Let the skeleton Σ be the six carbon atom ring of benzene. According to [3, VI], the group G of substitution isomerism of benzene has the following elements:

$$(1),(123456),(135)(246),(14)(25)(36),(153)(264),(165432),$$

$$(13)(46),(12)(36)(45),(26)(35),(16)(25)(34),(15)(24),(14)(23)(56).$$

Clearly, G coincides with the dihedral group $D_6 = \langle r,s\rangle$, where $r = (123456)$, and $s = (13)(46)$.

Case 1. $\lambda = (4,2)$.

There are three isomeric forms of the di-substitution products of benzene, called *para*, *ortho*, and *meta* derivatives. Therefore $N_{(4,2);\Sigma} = 3$, which is in agreement with the equality $n_{(4,2);G} = 3$.

We have $T_{(4,2);G} = \{a_{(4,2)}, b_{(4,2)}, c_{(4,2)}\}$, where:

$a_{(4,2)}$ is the G-orbit

$$\{(\{2,3,5,6\},\{1,4\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,3,4,6\},\{2,5\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,2,4,5\},\{3,6\},\emptyset,\emptyset,\emptyset,\emptyset)\}$$

of the tabloid $A^{(4,2)} = (\{2,3,5,6\},\{1,4\},\emptyset,\emptyset,\emptyset,\emptyset)$;

$b_{(4,2)}$ is the G-orbit

$$\{(\{1,2,3,4\},\{5,6\},\emptyset,\emptyset,\emptyset,\emptyset),(\{2,3,4,5\},\{1,6\},\emptyset,\emptyset,\emptyset,\emptyset),(\{3,4,5,6\},\{1,2\},\emptyset,\emptyset,\emptyset,\emptyset),$$

$$(\{1,4,5,6\},\{2,3\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,2,5,6\},\{3,4\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,2,3,6\},\{4,5\},\emptyset,\emptyset,\emptyset,\emptyset)\}$$

of the tabloid $B^{(4,2)} = (\{1,2,3,4\},\{5,6\},\emptyset,\emptyset,\emptyset,\emptyset)$;

$c_{(4,2)}$ is the G-orbit

$$\{(\{2,4,5,6\},\{1,3\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,3,5,6\},\{2,4\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,2,4,6\},\{3,5\},\emptyset,\emptyset,\emptyset,\emptyset),$$

$$(\{1,2,3,5\},\{4,6\},\emptyset,\emptyset,\emptyset,\emptyset),(\{2,3,4,6\},\{1,5\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,3,4,5\},\{2,6\},\emptyset,\emptyset,\emptyset,\emptyset)\}$$

of the tabloid $C^{(4,2)} = (\{2,4,5,6\},\{1,3\},\emptyset,\emptyset,\emptyset,\emptyset)$.

Case 2. $\lambda = (3^2)$.

The tri-substitution products of benzene exist in three isomeric forms if all the substituents are the same. They are known as *asymmetrical*, *vicinal*, and *symmetrical* derivatives. Thus $N_{(3^2);\Sigma} = 3$, which agrees with $n_{(3^2);G} = 3$.

We have $T_{(3^2);G} = \{a_{(3^2)}, b_{(3^2)}, c_{(3^2)}\}$, where:

$a_{(3^2)}$ is the G-orbit

$$\{(\{1,2,4\},\{3,5,6\},\emptyset,\emptyset,\emptyset,\emptyset),(\{2,3,5\},\{1,4,6\},\emptyset,\emptyset,\emptyset,\emptyset),(\{3,4,6\},\{1,2,5\},\emptyset,\emptyset,\emptyset,\emptyset),$$

$$(\{1,4,5\},\{2,3,6\},\emptyset,\emptyset,\emptyset,\emptyset),(\{2,5,6\},\{1,3,4\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,3,6\},\{2,4,5\},\emptyset,\emptyset,\emptyset,\emptyset),$$

$(\{2,3,6\},\{1,4,5\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,2,5\},\{3,4,6\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,4,6\},\{2,3,5\},\emptyset,\emptyset,\emptyset,\emptyset),$

$(\{3,5,6\},\{1,2,4\},\emptyset,\emptyset,\emptyset,\emptyset),(\{2,4,5\},\{1,3,6\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,3,4\},\{2,5,6\},\emptyset,\emptyset,\emptyset,\emptyset)\}$

of the tabloid $A^{(3^2)} = (\{1,2,4\},\{3,5,6\},\emptyset,\emptyset,\emptyset,\emptyset)$;
$b_{(3^2)}$ is the G-orbit

$\{(\{1,2,3\},\{4,5,6\},\emptyset,\emptyset,\emptyset,\emptyset),(\{2,3,4\},\{1,5,6\},\emptyset,\emptyset,\emptyset,\emptyset),(\{3,4,5\},\{1,2,6\},\emptyset,\emptyset,\emptyset,\emptyset),$

$(\{4,5,6\},\{1,2,3\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,5,6\},\{2,3,4\},\emptyset,\emptyset,\emptyset,\emptyset),(\{1,2,6\},\{3,4,5\},\emptyset,\emptyset,\emptyset,\emptyset)\}$

of the tabloid $B^{(3^2)} = (\{1,2,3\},\{4,5,6\},\emptyset,\emptyset,\emptyset,\emptyset)$;
$c_{(3^2)}$ is the G-orbit

$$\{(\{1,3,5\},\{2,4,6\},\emptyset,\emptyset,\emptyset,\emptyset),(\{2,4,6\},\{1,3,5\},\emptyset,\emptyset,\emptyset,\emptyset)\}$$

of the tabloid $C^{(3^2)} = (\{1,3,5\},\{2,4,6\},\emptyset,\emptyset,\emptyset,\emptyset)$.
Since $A^{(3^2)} < (135)(246)A^{(4,2)}$, $A^{(3^2)} < B^{(4,2)}$, $A^{(3^2)} < (135)(246)C^{(4,2)}$, $B^{(3^2)} < B^{(4,2)}$, $B^{(3^2)} < (14)(25)(36)C^{(4,2)}$, and $C^{(3^2)} < (123456)C^{(4,2)}$, we have

$$a_{(3^2)} < a_{(4,2)},\ a_{(3^2)} < b_{(4,2)},\ a_{(3^2)} < c_{(4,2)},$$

$$b_{(3^2)} < b_{(4,2)},\ b_{(3^2)} < c_{(4,2)},\ c_{(3^2)} < c_{(4,2)}.$$

The diagrams below represent the Körner relations between di- and tri-substitution products of benzene, which serve for complete identification of these six derivatives.

$$\begin{array}{c} a_{(4,2)} \\ \downarrow \\ a_{(3^2)} \end{array} \qquad \begin{array}{cc} & b_{(4,2)} \\ \swarrow & \downarrow \\ a_{(3^2)} & b_{(3^2)} \end{array} \qquad \begin{array}{ccc} & c_{(4,2)} & \\ \swarrow & \downarrow & \searrow \\ a_{(3^2)} & b_{(3^2)} & c_{(3^2)} \end{array}$$

Here the arrow $a \to b$ means that the isomers a and b are neighbours with $a > b$ and b can be obtained from a via a simple substitution reaction. The Körner's diagrams yield that $a_{(4,2)}$ represents the para compound, $b_{(4,2)}$ represents the ortho compound, $c_{(4,2)}$ represents the meta compound, $a_{(3^2)}$ represents the asymmetrical compound, $b_{(3^2)}$ represents the vicinal compound, and $c_{(3^2)}$ represents the symmetrical compound.

6.4. Here we shall discuss the derivatives of ethene, C_2H_4, and their genetic relations, taking into account the exposition from [3, VI]. The group G of substitution isomerism of ethene is the Klein subgroup of S_4:

$$G = \{(1),(12)(34),(13)(24),(14)(23)\}.$$

Since there are no chiral pairs, $G' = G$. For the group G'' we can choose any one of the three conjugated Sylow 2-subgroups of S_4, for instance

$$G'' = \{(1),(12)(34),(13)(24),(14)(23),(13),(24),(1234),(1432)\}.$$

The group G'' coincides with the dihedral group $D_4 = \langle r,s\rangle$, where $r = (1234)$, and $s = (13)$. Thus $r^2 = (13)(24)$, $r^3 = (1432)$, $sr = (12)(34)$, $sr^2 = (24)$, $sr^3 = (14)(23)$. These groups are defined in [3, VI] by using the inequalities (1.5.3) – (1.5.5).

The Abelian group G has four one-dimensional characters: The unit character, the character χ_1 with kernel $\langle(13)(24)\rangle$, the character χ_2 with kernel $\langle(12)(34)\rangle$, and the character χ_3 with kernel $\langle(14)(23)\rangle$.
Let Σ be the two carbon atom skeleton of ethene.
Case 1. $\lambda = (4)$.
Then $N_{(4);\Sigma} = n_{(4);G} = 1$, and $N''_{(4);\Sigma} = n_{(4);G''} = 1$.
We have $T_{(4);G} = T_{(4),G''} = \{a_{(4)}\}$, where $a_{(4)}$ is the only G-, and G''-orbit of the tabloid $A^{(4)} = (\{1,2,3,4\},\emptyset,\emptyset,\emptyset)$. The only G-orbit $a_{(4)}$ represents the parent substance of ethene.
Case 2. $\lambda = (3,1)$.
In this case, again $N_{(3,1);\Sigma} = n_{(3,1);G} = 1$, and $N''_{(3,1);\Sigma} = n_{(3,1);G''} = 1$.
We have $T_{(3,1);G} = T_{(3,1),G''} = \{a_{(3,1)}\}$, where $a_{(3,1)}$ is the only G-, and G''-orbit of the tabloid $A^{(3,1)} = (\{1,2,3\},\{4\},\emptyset,\emptyset)$. This is because both G, and G'' are transitive subgroups of S_4.
Moreover, $a_{(3,1)} < a_{(4)}$, since $A^{(3,1)} < A^{(4)}$.
Case 3. $\lambda = (2^2)$.
Then $N_{(2^2);\Sigma} = n_{(2^2);G} = 3$, and $N''_{(2^2);\Sigma} = n_{(2^2);G''} = 2$.
We have $T_{(2^2);G} = \{a_{(2^2)}, b_{(2^2)}, c_{(2^2)}\}$, where:
$a_{(2^2)}$ is the G-orbit

$$\{(\{1,2\},\{3,4\},\emptyset,\emptyset),(\{3,4\},\{1,2\},\emptyset,\emptyset)\}$$

of the tabloid $A^{(2^2)} = (\{1,2\},\{3,4\},\emptyset,\emptyset)$ with stabilizer $G_{A^{(2^2)}} = \langle(12)(34)\rangle$;
$b_{(2^2)}$ is the G-orbit

$$\{(\{1,4\},\{2,3\},\emptyset,\emptyset),(\{2,3\},\{1,4\},\emptyset,\emptyset)\}$$

of the tabloid $B^{(2^2)} = (\{1,4\},\{2,3\},\emptyset,\emptyset)$ with stabilizer $G_{B^{(2^2)}} = \langle(14)(23)\rangle$;
$c_{(2^2)}$ is the G-orbit

$$\{(\{1,3\},\{2,4\},\emptyset,\emptyset),(\{2,4\},\{1,3\},\emptyset,\emptyset)\}$$

of the tabloid $C^{(2^2)} = (\{1,3\},\{2,4\},\emptyset,\emptyset)$ with stabilizer $G_{C^{(2^2)}} = \langle(13)(24)\rangle$.
For the group G'', we have $T_{(2^2);G''} = \{u_{(2^2)}, v_{(2^2)}\}$, where:
$u_{(2^2)}$ is the G''-orbit

$$\{(\{1,2\},\{3,4\},\emptyset,\emptyset),(\{3,4\},\{1,2\},\emptyset,\emptyset),(\{1,4\},\{2,3\},\emptyset,\emptyset),(\{2,3\},\{1,4\},\emptyset,\emptyset)\}$$

of the tabloid $A^{(2^2)} = (\{1,2\},\{3,4\},\emptyset,\emptyset)$;
$v_{(2^2)}$ is the G''-orbit

$$\{(\{1,3\},\{2,4\},\emptyset,\emptyset),(\{2,4\},\{1,3\},\emptyset,\emptyset)\}$$

of the tabloid $C^{(2^2)} = (\{1,3\},\{2,4\},\emptyset,\emptyset)$.
Evidently, $u_{(2^2)} = a_{(2^2)} \cup b_{(2^2)}$, and $v_{(2^2)} = c_{(2^2)}$.
Moreover we have,

$$a_{(2^2)} < a_{(3,1)},\ b_{(2^2)} < a_{(3,1)},\ c_{(2^2)} < a_{(3,1)},$$

since $A^{(2^2)} < A^{(3,1)}$, $(13)(24)B^{(2^2)} < A^{(3,1)}$, and $C^{(2^2)} < A^{(3,1)}$, respectively.

Case 4. $\lambda = (2, 1^2)$.
Then $N_{(2,1^2);\Sigma} = n_{(2,1^2);G} = 3$, and $N''_{(2,1^2);\Sigma} = n_{(2,1^2);G''} = 2$.
We have $T_{(2,1^2);G} = \{a_{(2,1^2)}, b_{(2,1^2)}, c_{(2,1^2)}\}$, where:
$a_{(2,1^2)}$ is the G-orbit

$$\{(\{1,2\},\{3\},\{4\},\emptyset), \{(\{1,2\},\{4\},\{3\},\emptyset), (\{3,4\},\{1\},\{2\},\emptyset)\}, (\{3,4\},\{2\},\{1\},\emptyset)\}$$

of the tabloid $A^{(2,1^2)} = (\{1,2\},\{3\},\{4\},\emptyset)$ with stabilizer $G_{A^{(2,1^2)}} = \{(1)\}$;
$b_{(2,1^2)}$ is the G-orbit

$$\{(\{1,4\},\{2\},\{3\},\emptyset), \{(\{1,4\},\{3\},\{2\},\emptyset), (\{2,3\},\{1\},\{4\},\emptyset)\}, (\{2,3\},\{4\},\{1\},\emptyset)\}$$

of the tabloid $B^{(2,1^2)} = (\{1,4\},\{2\},\{3\},\emptyset)$ with stabilizer $G_{B^{(2,1^2)}} = \{(1)\}$;
$c_{(2,1^2)}$ is the G-orbit

$$\{(\{1,3\},\{2\},\{4\},\emptyset), \{(\{1,3\},\{4\},\{2\},\emptyset), (\{2,4\},\{1\},\{3\},\emptyset)\}, (\{2,4\},\{3\},\{1\},\emptyset)\}$$

of the tabloid $C^{(2,1^2)} = (\{1,3\},\{2\},\{4\},\emptyset)$ with stabilizer $G_{C^{(2,1^2)}} = \{(1)\}$.
For the group G'' we have $T_{(2,1^2);G''} = \{u_{(2,1^2)}, v_{(2,1^2)}\}$, where:
$u_{(2,1^2)}$ is the G''-orbit

$$\{(\{1,2\},\{3\},\{4\},\emptyset), (\{1,2\},\{4\},\{3\},\emptyset), (\{3,4\},\{1\},\{2\},\emptyset), (\{3,4\},\{2\},\{1\},\emptyset),$$
$$(\{1,4\},\{2\},\{3\},\emptyset), (\{1,4\},\{3\},\{2\},\emptyset), (\{2,3\},\{1\},\{4\},\emptyset), (\{2,3\},\{4\},\{1\},\emptyset)\}$$

of the tabloid $A^{(2,1^2)} = (\{1,2\},\{3\},\{4\},\emptyset)$;
$v_{(2,1^2)}$ is the G''-orbit

$$\{(\{1,3\},\{2\},\{4\},\emptyset), (\{1,3\},\{4\},\{2\},\emptyset), (\{2,4\},\{1\},\{3\},\emptyset), (\{2,4\},\{3\},\{1\},\emptyset)\}$$

of the tabloid $C^{(2,1^2)} = (\{1,3\},\{2\},\{4\},\emptyset)$.
Clearly, $u_{(2,1^2)} = a_{(2,1^2)} \cup b_{(2,1^2)}$, and $v_{(2,1^2)} = c_{(2,1^2)}$.
Moreover,

$$a_{(2,1^2)} < a_{(2^2)},\ b_{(2,1^2)} < b_{(2^2)},\ c_{(2,1^2)} < c_{(2^2)},$$

since $A^{(2,1^2)} < A^{(2^2)}$, $B^{(2,1^2)} < B^{(2^2)}$, $C^{(2,1^2)} < C^{(2^2)}$, and

$$a_{(2,1^2)} < a_{(3,1)},\ b_{(2,1^2)} < a_{(3,1)},\ c_{(2,1^2)} < a_{(3,1)}, \tag{6.4.1}$$

because $A^{(2,1^2)} < A^{(3,1)}$, $(12)(34)B^{(2,1^2)} < A^{(3,1)}$, and $C^{(2,1^2)} < A^{(3,1)}$.
Case 4. $\lambda = (1^4)$.
Then $N_{(1^4);\Sigma} = n_{(1^4);G} = 6$, and $N''_{(1^4);\Sigma} = n_{(1^4);G''} = 3$.
We have

$$T_{(1^4);G} = \{a_{(1^4)}, b_{(1^4)}, c_{(1^4)}, e_{(1^4)}, f_{(1^4)}, h_{(1^4)}\},$$

where:
$a_{(1^4)}$ is the G-orbit

$$\{(\{1\},\{2\},\{3\},\{4\}), (\{2\},\{1\},\{4\},\{3\}), (\{3\},\{4\},\{1\},\{2\}), (\{4\},\{3\},\{2\},\{1\})\}$$

of the tabloid $A^{(1^4)} = (\{1\},\{2\},\{3\},\{4\})$ (the right coset G of S_4 modulo G); $b_{(1^4)}$ is the G-orbit

$$\{(\{1\},\{2\},\{4\},\{3\}),(\{2\},\{1\},\{3\},\{4\}),(\{3\},\{4\},\{2\},\{1\}),(\{4\},\{3\},\{1\},\{2\})\}$$

of the tabloid $B^{(1^4)} = (\{1\},\{2\},\{4\},\{3\})$ (the right coset $G(34)$ of S_4 modulo G); $c_{(1^4)}$ is the G-orbit

$$\{(\{1\},\{4\},\{2\},\{3\}),(\{2\},\{3\},\{1\},\{4\}),(\{3\},\{2\},\{4\},\{1\}),(\{4\},\{1\},\{3\},\{2\})\}$$

of the tabloid $C^{(1^4)} = (\{1\},\{4\},\{2\},\{3\})$ (the right coset $G(243)$ of S_4 modulo G); $e_{(1^4)}$ is the G-orbit

$$\{(\{1\},\{3\},\{2\},\{4\}),(\{2\},\{4\},\{1\},\{3\}),(\{3\},\{1\},\{4\},\{2\}),(\{4\},\{2\},\{3\},\{1\})\},$$

of the tabloid $E^{(1^4)} = (\{1\},\{3\},\{2\},\{4\})$ (the right coset $G(23)$ of S_4 modulo G); $f_{(1^4)}$ is the G-orbit

$$\{(\{3\},\{1\},\{2\},\{4\}),(\{4\},\{2\},\{1\},\{3\}),(\{1\},\{3\},\{4\},\{2\}),(\{2\},\{4\},\{3\},\{1\})\},$$

of the tabloid $F^{(1^4)} = (\{3\},\{1\},\{2\},\{4\})$ (the right coset $G(132)$ of S_4 modulo G); $h_{(1^4)}$ is the G-orbit

$$\{(\{3\},\{2\},\{1\},\{4\}),(\{4\},\{1\},\{2\},\{3\}),(\{1\},\{4\},\{3\},\{2\}),(\{2\},\{3\},\{4\},\{1\})\},$$

of the tabloid $H^{(1^4)} = (\{3\},\{2\},\{1\},\{4\})$ (the right coset $G(13)$ of S_4 modulo G). For the group G'', we have

$$T_{(1^4);G''} = \{u_{(1^4)}, v_{(1^4)}, w_{(1^4)}\},$$

where: $u_{(1^4)}$ is the G''-orbit

$$\{(\{1\},\{2\},\{3\},\{4\}),(\{2\},\{1\},\{4\},\{3\}),(\{3\},\{4\},\{1\},\{2\}),(\{4\},\{3\},\{2\},\{1\}),$$

$$(\{3\},\{2\},\{1\},\{4\}),(\{4\},\{1\},\{2\},\{3\}),(\{1\},\{4\},\{3\},\{2\}),(\{2\},\{3\},\{4\},\{1\})\},$$

of the tabloid $A^{(1^4)} = (\{1\},\{2\},\{3\},\{4\})$ (the right coset G'' of S_4 modulo G''); $v_{(1^4)}$ is the G''-orbit

$$\{(\{1\},\{2\},\{4\},\{3\}),(\{2\},\{1\},\{3\},\{4\}),(\{3\},\{4\},\{2\},\{1\}),(\{4\},\{3\},\{1\},\{2\}),$$

$$(\{1\},\{4\},\{2\},\{3\}),(\{2\},\{3\},\{1\},\{4\}),(\{3\},\{2\},\{4\},\{1\}),(\{4\},\{1\},\{3\},\{2\})\},$$

of the tabloid $B^{(1^4)} = (\{1\},\{2\},\{4\},\{3\})$ (the right coset $G''(34)$ of S_4 modulo G''); $w_{(1^4)}$ is the G''-orbit

$$\{(\{1\},\{3\},\{2\},\{4\}),(\{2\},\{4\},\{1\},\{3\}),(\{3\},\{1\},\{4\},\{2\}),(\{4\},\{2\},\{3\},\{1\}),$$

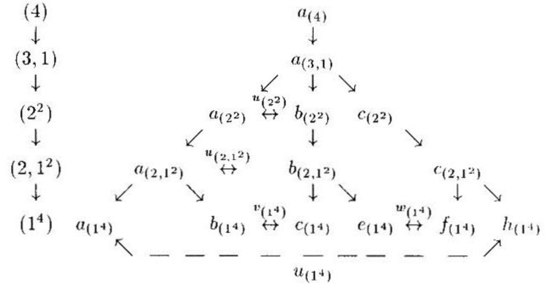
$$(\{3\},\{1\},\{2\},\{4\}),(\{4\},\{2\},\{1\},\{3\}),(\{1\},\{3\},\{4\},\{2\}),(\{2\},\{4\},\{3\},\{1\})\}.$$

of the tabloid $E^{(1^4)} = (\{1\},\{3\},\{2\},\{4\})$ (the right coset $G''(23)$ of S_4 modulo G'').
Clearly, $u_{(1^4)} = a_{(1^4)} \cup h_{(1^4)}$, $v_{(1^4)} = b_{(1^4)} \cup c_{(1^4)}$, $w_{(1^4)} = e_{(1^4)} \cup f_{(1^4)}$.
Further we have

$$a_{(1^4)} < a_{(2,1^2)},\ b_{(1^4)} < a_{(2,1^2)},\ c_{(1^4)} < b_{(2,1^2)},$$

$$e_{(1^4)} < b_{(2,1^2)},\ f_{(1^4)} < c_{(2,1^2)},\ h_{(1^4)} < c_{(2,1^2)},$$

because $A^{(1^4)} < A^{(2,1^2)}$, $B^{(1^4)} < A^{(2,1^2)}$, $C^{(1^4)} < B^{(2,1^2)}$, $(14)(23)E^{(1^4)} < B^{(2,1^2)}$, $F^{(1^4)} < C^{(2,1^2)}$, and $H^{(1^4)} < C^{(2,1^2)}$.
Here is the diagram which represents the derivatives of ethene.



The arrow $a \to b$ means that the isomers a and b are neighbours with $a > b$ and b can be obtained from a via a simple substitution reaction. The horizontal double arrow means that the two isomers are diastereomers and the letter above/below it denotes the corresponding structural isomer. The above diagram does not indicates the simple substitution reactions from (6.4.1), where the isomers are not neighbours.
Our extended approach confirms the conclusion of Lunn and Senior from [3, VI] that there are no type properties which distinguish the members of the pairs of diastereomers $a_{(2^2)}, b_{(2^2)}$ and $a_{(2,1^2)}, b_{(2,1^2)}$. It is clear that the genetic relations from the above diagram fail to make any difference between them. On the level of one-dimensional characters of the group G, the members of the second pair are indistinguishable because the stabilizers of their elements coincide with the unit group. At first sight each one of the characters χ_2 and χ_3 of the group G "distinguishes" $a_{(2^2)}$ and $b_{(2^2)}$: For instance χ_2 is identically 1 on the stabilizer $G_{A^{(2^2)}} = \langle(12)(34)\rangle$ of the tabloid $A^{(2^2)} \in a_{(2^2)}$ and χ_2 is not identically 1 on the stabilizer $G_{B^{(2^2)}} = \langle(14)(23)\rangle$ of the tabloid $B^{(2^2)} \in b_{(2^2)}$. The same is true for χ_3 if we replace $a_{(2^2)}$ for $b_{(2^2)}$ and vice versa. It is not hard to check that the presence of a non-trivial one-dimensional character θ of $S_{(2^2)}$ in the formula (5.1.2) has the same effect as the interchange of χ_2 and χ_3. Unfortunately, the characters χ_2 and χ_3 can not be distinguished: Each one of them can be obtained from the other by a special automorphism of the group G, that is induced by a renumbering the unsatisfied valences of the skeleton Σ. Therefore we can only conclude that both $a_{(2^2)}$ and $b_{(2^2)}$ are elements of the symmetric difference

$$(T_{(2^2);\chi_2} \backslash T_{(2^2);\chi_3}) \cup (T_{(2^2);\chi_3} \backslash T_{(2^2);\chi_2}),$$

so the type properties corresponding to χ_2 and χ_3 via the Extended Lunn-Senior Thesis 1.6.1 can not be used to make difference between the members of this pair of diastereomers. Thus, "...Whenever diameric pairs of disubstitution derivatives of ethylene have been investigated, it has been necessary to fall back on the specific properties of the molecules in question in order to decide which one is the cis and which one the trans isomer" (see [3, VI]).

Resume of Part I

There are four themes in this paper, which may be of interest to a chemist:
1) The determination of the structural formula of a potentially existing isomer with given skeleton Σ, starting from any tabloid in the symmetry group's orbit which represents this isomer according to Lunn-Senior thesis 1.5.1;
2) the partial order $\leq$ on the set of all G-orbits of tabloids (Section 4 and the subsidiary Sections 1 - 3);
3) the hypothesis that the set of (χ, θ)-orbits determines a type property of the molecule under consideration (Section 1, 1.6.1), and the count of (χ, θ)-orbits (Section 5);
4) the attempt to breathe new life into the philosophy of the original Lunn-Senior's paper [3].
Below, all isomers in a particular consideration have the same skeleton Σ.
The way of construction of the structural formula of an isomer is explicitly build in the representation of this isomer by a tabloid $A = (A_1, A_2, \ldots)$: If $i \in A_k$, then we attach the univalent substituent x_k to Σ's unsatisfied valence number i, for $k = 1, 2, \ldots$. Since there is no "canonical" numbering of the unsatisfied valences, a main problem of the present model is the identification of the real substances (if any) having these structural formulae, in terms of the model itself. The partial order $\leq$, and the (χ, θ)-orbits can be applied for this problem to be solved (at least partially).
The partial order may also be used in the following way:
The relation $a < b$ between the isomers a and b is an indication of the existence of a finite sequence of simple substitution reactions $b \to c_1 \to \cdots \to c_r \to a$, where the compounds $c_1, \ldots, c_r$, are intermediate stages in a synthesis of a. Such a sequence $c_1, \ldots, c_r$ (which is far-away of being unique), can be constructed by means of Theorem 3.4.4.
The relation $a \not\leq b$ implies that the isomer a for sure can not be obtained from the isomer b via a finite sequence of simple substitution reactions.
The partial order is tested in Section 6 for finding the genetic relations of the substitution derivatives of ethene. It is applied also in the case of di-, and tri-substitution derivatives of benzene and yields the classical Körner's relations. These two applications are considered also in Lunn-Senior's paper, Part VI. It goes without saying that the adequacy of this partial order to the chemical reality needs more experimental verifications.
A central topic in the paper is a detailed study of the notion of "neighbourhood" with respect to the above partial order. If two isomers a and b are neighbours with $a < b$, then probably there exists a chemical reaction $b \to a$, but it is certain that this reaction can not be represented as $b \to c \to a$, where c is a isomer. The main result in this direction is Theorem 4.2.3, (ii), which characterizes mathematically the pairs of neighbours $a < b$, and in this case predicts the existence of a chain $b \to c_1 \to \cdots \to c_r \to a$, where the intermediate "reactions" are "virtual", that is, $c_1, \ldots, c_r$ are not represented by tabloids, but by ordered dissections.

Item 5 of the Extended Lunn-Senior Thesis 1.6.1 is our hypothesis. If χ is a one-dimensional character of the symmetric group G of the molecule, and if θ is a one-dimensional character of the group S_λ (this group reflects the empirical formula (1.1.2) of the molecule), then the couple (χ, θ) produces via condition (5.1.3) a subset of the set of all G-orbits, which, we suppose, represents a type property of this molecule. This is true when $\chi = 1_G$, and $\theta = 1_{S_\lambda}$. In this particular case we obtain the set of all G-orbits, each one of them possibly representing an isomer due to Lun-Senior Thesis 1.5.1. This also is true in case $\chi = \chi_e$, and $\theta = 1_{S_\lambda}$ (see Section 6, 6.1), and we get a set which represents the chiral pairs. Theorem 5.3.1 is a wide generalization of a crucial result of Ruch (see Theorem 6.2.1) which connects the existence of chiral pairs with the dominance order among the partitions. This theorem holds out a hope that the Extended Lunn-Senior Thesis 1.6.1 is valid. Which couples (χ, θ) are within the scope of 1.6.1, item 5, is a matter of the experiment. We guess that there are no exceptions. Theorem 5.2.7 gives an explicit formula for the number of the (χ, θ)-orbits.

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