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Algebraic Combinatorics in Mathematical Chemistry. Methods and Algorithms. I. Permutation Groups and Coherent (Cellular) Algebras

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TUM-M9510

Dezember 95

Technische Universität München

Cataloging Data :
M. Klin, Ch. Rücker, G. Rücker, G. Tinhofer: Algebraic Combinatorics in Mathematical Chemistry. Methods and Algorithms. I. Permutation Groups and Coherent (Cellular) Algebras; Techn. Univ. München, Fak. f. Math, Report TUM M9510 (95)

Mathematics Subject Classification : 05C25 05C60 05E99

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Algebraic Combinatorics in Mathematical Chemistry. Methods and Algorithms. I. Permutation Groups and Coherent (Cellular) Algebras.

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Abstract.

Let (G,Ω) be a permutation group of degree n. Let $V(G,\Omega)$ be the set of all square matrices of order n which commute with all permutation matrices corresponding to permutations from (G,Ω). $V(G,\Omega)$ is a matrix algebra which is called the centralizer algebra of (G,Ω). In this paper we introduce the combinatorial analogue of centralizer algebras, namely coherent (cellular) algebras and consider the properties of these algebras. It turns out that coherent algebras provide a very helpful tool for the investigation of the symmetries of graphs of different kinds, in particular, of molecular graphs.

[1] Partially supported by DAAD allowance for study visit to Germany

[2] Supported by grant #I-0333-263.06/93 from the G. I.F. , the German-Israeli Foundation for Scientific Research and Development

Contents

1 Introduction

1.1. *Mathematical chemistry* was developed as a new area of science during the last decades. The term mathematical chemistry appears also in the names of an international scientific society, international conferences, journals, etc. This is justification enough for its general use. However, the subject of mathematical chemistry is still not well–defined. Just as "mathematical physics" and "applications of mathematics in physics" are not synonyms, mathematical chemistry is not simply "application of mathematical tools" to problems in chemistry.

In our opinion, the kernel of mathematical chemistry is associated with mathematical modelling in structural chemistry (in particular organic as well as stereochemistry) and with methods and algorithms for the solution of problems which appear in the course of gaining, processing and manipulating information about chemical structures and reactions.

Molecular design, computer synthesis of molecular structures, chemical informatics, investigation of structure–activity relationships (QSAR), expert systems, and other artificial intelligence applications in chemistry – all these areas of activity require the systematic use of "non–numerical procedures" such as combinatorical exhaustive search, algebraic transformations, logical deduction, processing of lists of symbols, etc. For this reason, mathematical tools from graph theory, group theory, algebraic combinatorics, discrete geometry, logical programming and from other branches of mathematics play a significant role in the creation of mathematical chemistry.

1.2. The *structural formula* (*constitutional formula*) of a compound is certainly the main tool in modelling chemical isomers. For mathematicians, it describes a colored multigraph. For this reason, identification of graphs and description of their symmetry properties are subjects of joint interest for chemists and mathematicians. Moreover, investigation of chemical graphs was one of the most productive points in the development of early graph theory (as it was conclusively shown in [BigLW76]). On the other hand, at the early stage of creating structural notions, chemists prefered to use clear and simple graph–theoretic notations (see brief historical surveys in [KerLM90], [RanT94]). Unfortunately, this initial harmony between chemists and mathematicians (for impressive examples see [Cru864] and [Syl878]) did not survive for a significantly long period of time.

In spite of the continuous existence of many productive interdisciplinary links created by the efforts of several bright persons acting in both areas of science, at the beginning of our century graph theory and structural chemistry started to develop independently.

1.3. With the outset of the computer era new technology was required also in chemistry. One of the first answers to this need was given by H. L. Morgan in [Mor65]. He introduced what a mathematician would call a stabilization procedure for finding the automorphism partition of the vertices of a graph (the notation used here is explained in subsequent sections). At the same the time first publications on graph isomorphism recognition appeared in mathematical journals, more or less independently, for example [Ung64], [Tur68], [Sko69]. These and other publications suggested *heuristic* isomorphism algorithms. Also counterexamples for the correctness of such algorithms were presented in these papers. Within a few years the graph isomorphism problem became very fashionable. This fact created a peculiar situation which in [ReaC77] and [Gat79] was called "the graph isomorphism disease". [ReaC77] and [Gat79] are annotated bibliographies reporting on the state of the art at that time. To the credit of mathematicians, starting with the paper by Morgan, they felt responsible to be acquainted with all results in the area (independent of their mathematical or chemical origin).

1.4. Soon after the appearance of Morgan's paper several Soviet scientists (in particular, G.M. Adel'son–Vel'skiĭ and his students A.A. Leman and B. Yu. Weisfeiler) were attracted by the graph isomorphism problem. They generalized the original simple stabilization process and discovered its algebraic nature. Eventually, Weisfeiler and Leman introduced the new notion of *cellular algebra* which turned out to be extremely useful in the study of graph isomorphism. This notion is one of the central subjects of our paper.

Almost at the same time D.G. Higman introduced a similar notion and called it a *coherent configuration* [Hig70]. In matrix terminology, it is now called a *coherent algebra* [Hig87].

The first paper on cellular algebras [WeiL68] was written in a rather sophisticated manner. New attempts were undertaken in [Wei76] to create a more complete and friendly exposition. Nevertheless, during two decades the Weisfeiler–Leman approach was almost unknown beyond the former USSR. The language of coherent algebras became adopted in mathematics but remained unknown in chemistry.

1.5. As we intend to show in this and in subsequent papers, coherent (cellular) algebras play a crucial role in Algebraic Combinatorics, a new area of modern mathematics. Unfortunately, up to now, there is almost zero influence of this powerful mathematical subject on mathematical chemistry. In all "chemical" papers concerned with the identification and manipulation of chemical structures (see Section 3 for a brief survey) algebraic ideas related to cellular algebras are still not in use.

In our opinion, the most serious reason for this is a terrible lag of mathematical education of chemists, especially of organic chemists, behind modern requirements (briefly mentioned in Subsection 1.1). A prospective chemist in whatever country will learn a little bit Calculus and some fundamentals in Differential Equations Theory and Linear Algebra, but he will not become acquainted with (or will be left having serious gaps in) the foundations of Set Theory and Mathematical Logics, Group Theory and Discrete Mathematics.

The mathematical community, too, shares responsibility for the increasing disproportion between the powerful abilities of modern mathematics and the non-satisfactory level of their use in other areas of science. In particular, there is still no friendly and detailed self-contained introduction to coherent (cellular) algebras available for a wide chemical community. Several survey papers written by Western and Soviet mathematicians, see

Section 10, are oriented only towards experts in mathematics.

1.6. It is our first and deliberately chosen aim to fill this gap. The present paper is the first in a planned series. For this reason, it is mostly of an expository nature. However, it will create the background necessary for the understanding of new applications in mathematical chemistry which will be described starting with the second paper in the series.

Those who are chemists by training will find in the paper a reasonable amount of motivation, arguments and examples related to chemistry. We hope that this chemical material will permanently maintain their attention to the topic. However, our style of exposition follows mostly the standards of teaching mathematical material, hence, we suppose from the beginning the presence of sufficient initial interest to a new chapter of mathematics. Thus we do not always try to create immediate rewards for the patience and openness of the reader.

We hope also that the paper will be a helpful introduction to applied algebraic combinatorics for students and professionals in discrete mathematics, independently of their acquaintance with chemistry.

1.7. It is worthwhile to mention that each of the authors has followed his own complicated way to our joint subject.

M. Klin developed in 1969 - 1974 (partly in joint work with L. A. Kalužnin) a general scheme for the use of Galois correspondences in the investigation of overgroups of a given permutation group, as well as for the enumeration of graphs with a prescribed automorphism group, see [Kli70a], [Kli70b], [Kli72], [KalK72], [Kli74].

G. Tinhofer in 1974 - 1977 worked out (partly in joint work with his student J. Hinteregger) an approach to graph stabilization which is equivalent to the cellular algebra approach, see [Tin75], [Tin76], [HinT77]. In spite of the fact that this approach was discussed in [Gat79], these papers are still almost unknown even to experts in algebraic combinatorics.

Ch. Rücker and G. Rücker (a chemist and a mathematician by education) perhaps were the first in chemistry to apply a matrix stabilization procedure for the perception of symmetry and isomorphism of graphs in the course of their work on computer generation of IUPAC nomenclature for chemical graphs, see [RueR90a], [RueR90b], [RueR91a], [RueR91b].

Starting in 1990, acquaintance between the authors was built up stepwise, first by communication and then personally. During nine years all of us made a lot of steps in order to achieve a common understanding in chemistry and mathematics. This paper is in fact the product of a long "friendly struggle", interchange of ideas and mutual compromises in the elaboration of a suitable style of the presentation. Therefore we hope that the paper will serve as a complete, self–contained, friendly and helpful introduction to the algebraic point of view to the problems of graph symmetry perception.

1.8. We did our best to load the text with a large number of examples which will serve the reader as a guide on his long travel to the country of algebraic combinatorics. Our presentation is rather elementary, we avoid proofs and the overuse of abstract notions. Sometimes the discussion of details is deliberately postponed to further papers of the series (for example, a full description of the Weisfeiler–Leman stabilization will be the subject of the second paper). However, a reader who considers mathematics only as a source of immediately working prescriptions perhaps will be disappointed by our "slow" speed of presentation. Applications to real problems in chemistry will not appear before the end of the paper in Section 9. Discussion of actual algorithms, disproof of naive conjectures related to stabilization, discussion of practically efficient methods for graph identification and perception of graph symmetry, comparison and "competition" of classical heuristics with rigorous procedures will be certainly the subject of our considerations, but only in future papers of the series.

1.9. Let us add some words about the structure of the paper. Informally, it can be divided into four parts.

Part 1 consists of Sections 1–3, it can be considered as a comprehensive introduction. For this reason, the presentation in this part is plain text. Here we deliberately avoid rigorous formulations.

Part 2 consisting of Sections 4–6 is the crucial part of the paper. Here the knowledge of permutation groups, centralizer rings and cellular algebras is introduced. The reader has to understand everything in this part, otherwise he will not be able to follow the further parts.

Part 3 consists of Sections 7–9 and contains rather abstract mathematical material. A reader who is not educated sufficiently in mathematics, as it may happen with a chemist, perhaps will not be able to digest this part at the first reading. However, we urge everybody to display patience and persistence: after a few serious attempts the main ideas will become clear, and then the content of this part will create additional insight into the material and explain the connections between the notions introduced in Part 2.

Part 4 consists of Section 10 and the bibliography. Some historical remarks and some comments on the content of our intended subsequent papers will broaden the reader's outlook and will help to find an independent way to articles and books which treat the presented material more deeply and widely.

1.10. In principle, no fundamental mathematical education is necessary for the understanding of this paper. Hence, we hope that the paper is useful for every chemist who has acquired a certain experience of dealing with mathematical literature. However, we have to suppose acquaintance with certain elementary prerequisites. For example, notions and notations related to sets such as subset, element of a set, inclusion, are used without any explanation. Also a knowledge of basic terms in graph theory is of advantage but not obligatory. In case of any misunderstanding the reader may consult one of the standard textbooks in graph theory, e.g. [Har69], [Big85]. Acquaintance with elementary linear algebra is supposed, at least at the level of matrix manipulation.

All fundamentals of group theory which are necessary for the reading of the paper will be developed in Section 4. However, several times we appeal to the knowledge of classical crystallographic point groups which we consider as a traditional obligatory element of a chemist's mathematical training.

2 The subject of algebraic combinatorics

2.1. *Combinatorics* is a part of mathematics which deals with various structured objects called *combinatorial objects*: graphs, hypergraphs, designs, finite geometries, etc. In this context combinatorial object is a basic notion. It can be rigorously defined by set-theoretical means using the notions of "subset", "cartesian product of sets" and "function between finite sets". One of several attempts to formalize the notion of combinatorial objects was undertaken in [KalP86]. A similar approach based on the use of a "ladder of combinatorial objects" was set up in [TraZ87], [Tra95] in order to formalize "chemical combinatorial objects" for the purpose of structural organic chemistry. In this paper we restrict ourselves to the consideration of graphs and some of their modifications.

2.2. Let us start with the notion of a simple (undirected) graph (a rigorous and general definition is given in 4.17).
A *graph* $\Gamma = (V, E)$ consists of a set V of *vertices* and a set E of *edges*, where E is a subset of $\left\{ V \atop 2 \right\}$, the set of all 2-element subsets of V. If $e \in E$ and $e = \{x, y\}$, then the vertices x and y are called *endpoints* of e, e is *incident* with x and y, and x and y are *adjacent* (or *joined* by the edge e).

The *valency* or *degree* of a vertex x is the number of edges incident with x. The graph Γ is called *regular* of *valency* r, if each vertex has valency r.

A graph can be represented by means of a list ("connection table"), a diagram or an adjacency matrix (see Sections 4–5 for details). In a *diagram*, vertices are usually represented by small circles (or by bold dots), while edges are depicted by line segments or arcs joining their endpoints.

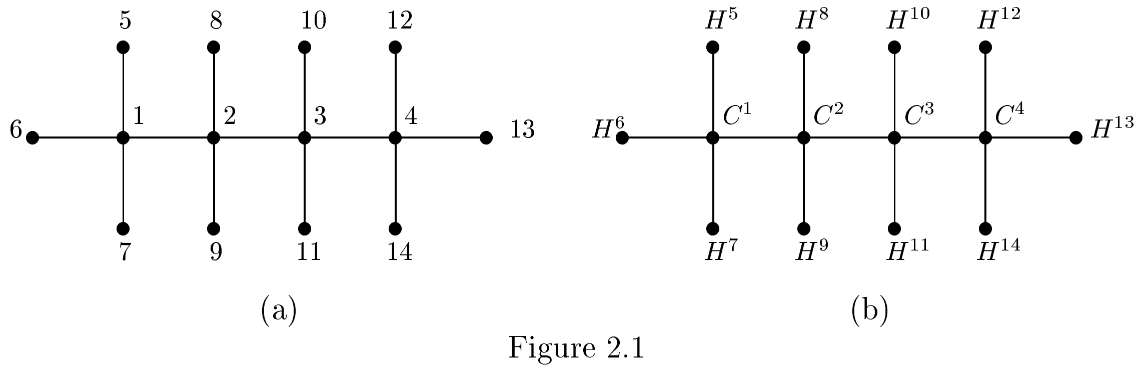


Figure 2.1

In order to distinguish vertices, we can associate *labels* to some or to all of them (different vertices get different labels), such a graph is called a *labelled graph*. Moreover, we can associate additional labels of another kind to vertices and also to edges. Such labels are often called *colors*. They need not be different for different vertices or for different edges. For convenience, as a rule, labels for vertices will be natural numbers. Colors for vertices and edges in mathematical chemistry can carry chemical information (type of atom or bond).

2.3. Example. Figure 2.1a represents a labelled graph, while Figure 2.1b shows a colored labelled chemical graph representing the structural formula of n-butane. The superscripts at the atom symbols are the conventional labels of the corresponding vertices in Figure 2.1a.

2.4. Let V, V' be two sets, and let $g : V \longrightarrow V'$ be a mapping which assigns to each element $x \in V$ an element $x' \in V'$. We shall write $x' = x^g$ in order to express that x' is the *image* of x under the mapping g. The mapping g is called a *one–to–one correspondence on* or a *bijection between* V and V' if

(i) different elements from V get different images and

(ii) each element x' from V' is the image of some element in V.

Two graphs $\Gamma = (V, E)$ and $\Gamma' = (V', E')$ are called *isomorphic* if there exists a bijection g between V and V' which preserves adjacency of vertices. If this happens then g is called an isomorphism from Γ to Γ'. In other words, a bijection g is an isomorphism from Γ to Γ' if and only if for each edge $e = \{x, y\}$ of Γ its image $e^g = \{x^g, y^g\}$ is an edge of Γ' and each edge e' of Γ' is the image of some edge e of Γ. Roughly speaking, isomorphic graphs are distinct only in their labeling. The class of all graphs which are mutually isomorphic and which are non-isomorphic to every graph not contained in that class is called an *isomorphism class* of graphs or an *abstract graph*. An abstract graph can be thought of as the prototype of a certain structure, each particular graph in the class is a *representative* of this structure.

The *graph isomorphism problem* (the problem of recognizing whether two graphs Γ and Γ' are isomorphic or not) is non-trivial, even for relatively small graphs which can be depicted by diagrams.

2.5. Example. Figure 2.2 shows diagrams of eight labeled regular graphs of valency 3. Each of them has 8 vertices. Recognize which graphs are isomorphic.

Note that the graphs Γ_1 and Γ_5 are identical, they have the same vertex set and the same edge set. Hence for these two graphs the essence of the isomorphism problem is rather artificial. It is related only to the different geometrical view of the corresponding diagrams. The diagram of Γ_5 is *plane*, i.e. edges intersect only at their end points if at all. The diagram of Γ_1 is not plane.

For all other pairs of graphs in Figure 2.2 the solution of the isomorphism problem is not so evident. First we can distinguish obviously non-isomorphic pairs. Γ_6 and Γ_8 are the only graphs which include triangles, hence they cannot be isomorphic to any of the other six graphs. Γ_2 and Γ_7 possess cycles of length 5, while such cycles cannot be found (and we have to prove this) in $\Gamma_1, \Gamma_3, \Gamma_4$ and Γ_5. Hence, Γ_2 and Γ_7 are candidates to be isomorphic graphs. To confirm this, we have to establish an actual isomorphism. For example

$$g = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 1 & 3 & 5 & 7 & 2 & 4 & 6 & 8 \end{pmatrix}$$

is an isomorphism from Γ_2 to Γ_7. In this notation for g the arguments x are listed in the first row while the corresponding images x^g are given in the second row. If the bijection g is given as "Deus ex machina" then there is no problem to check that g indeed represents an isomorphism. However, up to the moment, the only generally applicable way to find a suitable permutation for representing an isomorphism is a more or less complete search through all $8! = 40320$ possible bijections. We suggest to the reader to prove that for example Γ_1 and Γ_4 are isomorphic, and hence, are different representatives of the same abstract graph.

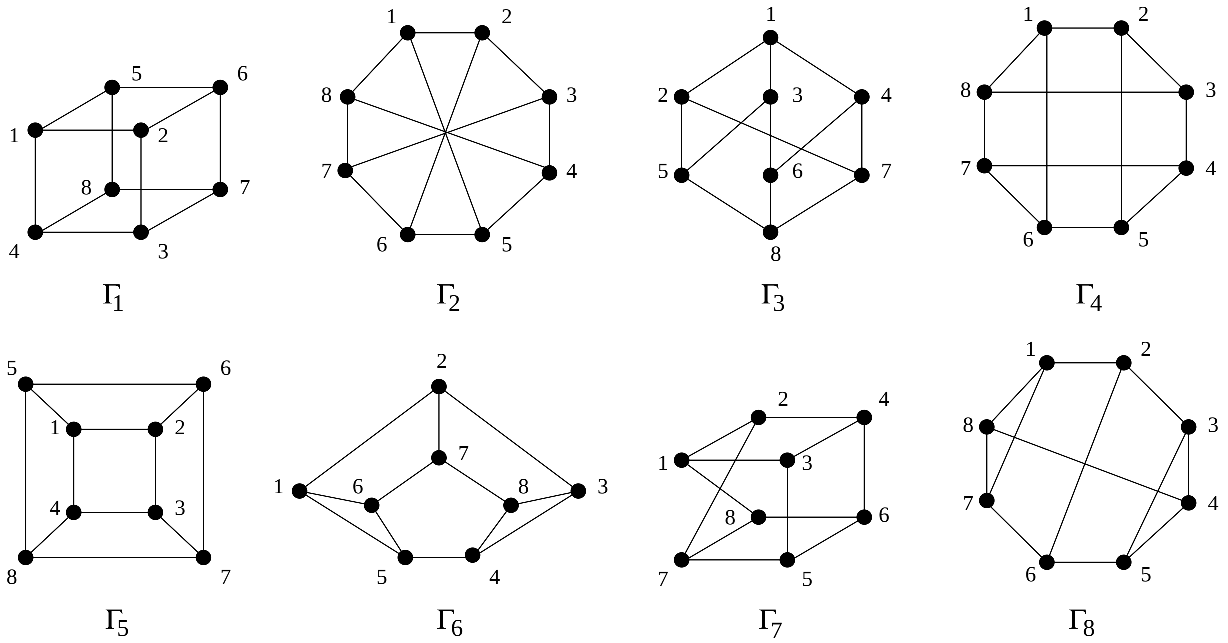


Figure 2.2.

2.6. According to the well-known Stirling formula (see, e.g. [Fel57])

$$n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n,$$

in general, a complete direct search for the solution of the isomorphism problem for two graphs with n vertices requires exponential time, i.e. a number of operations exponentially increasing for increasing n. During the last three decades numerous rigorous as well as heuristic strategies were established and implemented in order to avoid complete search in isomorphism testing. Some of them will be discussed in subsequent sections of this paper and in subsequent papers of this series. For restricted classes of graphs these strategies can be successful. However, in general, whether there exists an algorithm for isomorphism testing which runs in polynomial time is still an open problem. Moreover, this question is considered as one of the most challenging problems in graph theory.

2.7. An isomorphism of graph $\Gamma = (V, E)$ with itself is called an *automorphism* of Γ. Let $Aut(\Gamma)$ denote the set of all automorphisms of Γ. It turns out that $Aut(\Gamma)$ together with the operation of the superposition (muliplication) of bijections satisfies all the axioms which define a special algebraic structure called a *group* (see Section 4). Hence, $Aut(\Gamma)$ is called the *automorphism group* of Γ.

To describe all symmetries of a graph means to find all its automorphisms. In mathematics special attention has been paid to graphs with high symmetry. The level of symmetry of a graph can be described in terms of the action of $Aut(\Gamma)$ on its elements of a prescribed kind: vertices, edges, non-edges, cycles of given length, etc. For example, a graph Γ is called *vertex–transitive*, if all vertices are equivalent with respect to the action of $Aut(\Gamma)$, i.e. if for each pair $x, y \in V$ there is a $g \in Aut(\Gamma)$ such that $y = x^g$. Every vertex–transitive graph is regular, the opposite claim is not true. For example, in subsequent sections we shall show that the graphs Γ_6 and Γ_8 of Example 2.5 (which are, in fact, isomorphic) are not vertex-transitive, while all other graphs in this example are vertex–transitive.

2.8. The investigation of highly symmetric graphs was the starting point of Algebraic Combinatorics.

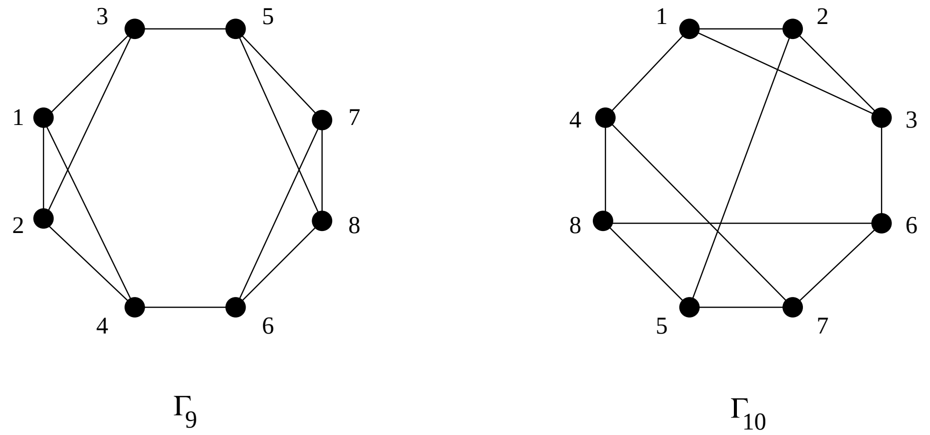


Figure 2.3.

As a typical example of such a problem let us consider the problem of enumerating all cubic graphs , i.e. all graphs which are regular of valency 3 (see [BarF78]). It is evident that each cubic graph has an even number n of vertices. There exists exactly one cubic graph on $n = 4$ vertices, namely the complete graph K_4. It can be easily seen that there are exactly two non-isomorphic cubic graphs with $n = 6$. For $n = 8$ the problem is less trivial. According to [BarF78] there exist exactly five non-isomorphic connected cubic graphs with 8 vertices. Three of them can be found in Figure 2.2. The remaining two are depicted in Figure 2.3.

These two graphs, as well as Γ_6 and Γ_8, are not vertex–transitive. All connected cubic graphs with $n = 8$ are *hamiltonian*, i.e. contain a cycle passing through all vertices exactly once (see Figures 2.2 and 2.3). Further interesting graph-theoretical properties of 8-vertex connected cubic graphs are mentioned in [BarF78]. For example, exactly two of them are nonplanar, i.e. cannot be represented by a plane diagram. By the way, hydrocarbons corresponding to the planar graphs Γ_1, Γ_6 and Γ_9 have been synthesized, see [Eat92], [RueT88].

2.9. Now, let us define the problem of enumerating combinatorial objects with given properties (for example, with given values of certain parameters). We distinguish two kinds of enumeration: constructive and analytical enumeration.

Constructive enumeration means to construct a transversal of the set of all isomorphism classes of certain objects with given properties. A *transversal* includes one and only one representative of each isomorphism class. For instance, $\Gamma_1, \Gamma_2, \Gamma_6, \Gamma_9$ and Γ_{10} is a transversal of the isomorphism classes of connected cubic 8-vertex graphs.

For *analytical enumeration*, it suffices to know the size of a transversal or certain additional information about the number of objects in a transversal having prescribed values of other parameters. In our case, the number 5 is the result of the analytical enumeration of all connected cubic graphs of $n = 8$ vertices. Below we have listed the results of the analytical enumeration of such graphs for $n \leq 18$ (due to [BarF78]). The first line shows the number n, the second line the corresponding size t of a transversal:

Table 2.1:

n	4	6	8	10	12	14	16	18
t	1	2	5	19	85	509	4060	41301

In the same paper, the results of the constructive enumeration are also given for $n \leq 12$ (they occupy several pages). The complete results of constructive enumeration achieved as yet would fill a voluminous book.

2.10. Enumeration of graphs (analytical as well as constructive) was one of the origins of interest into graph theory from the point of view of mathematical chemistry. Several references will be briefly discussed in the next section. Here we only stress that enumeration of cubic graphs has a rather long history in mathematical chemistry, as well as in graph theory, see for example [Bal66], where all connected cubic 10-vertex graphs are constructed.

In mathematics enumeration of highly symmetric graphs is regarded as part of the classification problem. From the beginning techniques from group theory and linear algebra were used for the formulation of the problem as well as for its solution (see e.g. N. Biggs [Big74] who coined the term "algebraic graph theory").

In the course of the development of algebraic graph theory the following general strategy was applied. Suppose, we want to describe graphs of a given type of high symmetry.

Then we may start with some "combinatorial approximation" to this property which is easier to deal with. This means that we establish necessary conditions in terms of certain graph parameters. Then we investigate the wider class of graphs which satisfy these conditions. Thus, replacing the class of vertex-transitive graphs by regular graphs gives a naive example of such an approximation. Unfortunately, in this case, the approximation is not very successful. For example, only 5 out of the 41301 connected cubic 18-vertex graphs are vertex-transitive (see [BarF78]). This shows that in general a combinatorial approximation has to be established on a deeper foundation.

2.11. One of the more successful approaches to combinatorial approximations, the theory of association schemes, helps to form the kernel of modern *Algebraic Combinatorics.* A brief survey of the initial notions of this theory, even in the more general framework of coherent (cellular) algebras, is presented in Sections 5–6. Historical comments will be found in Section 10. Here we only mention D.G. Higman and B.Yu. Weisfeiler & A.A. Leman as the founders of two simultaneous approaches to the investigation of those algebras. We also stress once more that one of the important stimuli for the creation of cellular algebras came from the problem of identification of molecular graphs.

2.12. In the preface of their book [BanI84], E. Bannai and T. Ito jocosely announce their intention to give a treatment of group theory without groups. In fact, they replace the centralizer algebras of permutation groups (in particular, of transitive permutation groups) by their combinatorial approximation, namely by coherent algebras (Section 6). One can state the axioms of coherent algebras without using group-theoretical notions. However, the use of cellular algebras helps (via the so-called Galois correspondences, see Section 7) to obtain new information about the whole symmetry of all graphs which are invariant with respect to a prescribed permutation group. Of course, at this moment not every reader will understand the essence of all links mentioned here. Anyway, please, consider this subsection as a brief outline of the bulk of material in this paper.

2.13. As stated in the introduction, algebraic combinatorics and mathematical chemistry have a rather long history of mutual fruitful influence in the course of their almost simultaneous development. Unfortunately, the theory of coherent algebras is still almost unknown to experts in mathematical chemistry. We intend to fill this gap and to introduce new ideas into the world of chemists investigating symmetry and identification problems of chemical graphs. Our series of papers is designed

- to introduce the reader to the theory of coherent algebras and its applications
- to describe systematically different approaches to graph stabilization (including program implementations of the classical Weisfeiler-Leman stabilization)
- to acquaint the reader with recent results in graph isomorphism theory
- to describe rigorous practically efficient graph isomorphism algorithms and algorithms for the construction of the automorphism group of graphs which are based on the combination of backtracking techniques with group-theoretical tools.

3 Problems related to the perception of the symmetry of chemical graphs

3.1. The traditional view of "symmetry through the eyes of a chemist" (title of the book [HarH86]) is based on geometry. Generally speaking, a molecule is regarded as a system of nuclei of atoms and an electron density distribution in 3D space. With 3D atom coordinates given, the symmetry of the molecule is represented by the symmetry of its geometry. The latter can be described in terms of transformations of the Euclidean space which preserve distances between points and angles between lines. For every molecule, there is a limited number of symmetry operations effecting this, which form a group in the mathematical sense, and this is where group theory traditionally enters chemistry. This view is very successful for numerous applications in physical and organic chemistry, as reflected in many textbooks, see for example [Cot90], [Wig59], [Sch65], [Hoc66], [Hal69], [Bis73], and others. In what follows we shall use the term "geometrical symmetry" for this classical approach.

However, in organic chemistry sometimes an even more abstract picture of a molecule is used, the constitutional formula, carrying information simply on which atom is related to which other atom by what type of bond, and neglecting any geometrical implications. This picture actually is a graph (an entity made of points (vertices) and lines (edges) connecting them), and graph theory therefore has its legitimate place in chemistry, see [Tri92], [BonR91]. Some of its major fields of application are listed below.

A graph, too, has its symmetry, for example two vertices may be equivalent with respect to their relations to the remainder of the graph. In mathematical chemistry, this kind of symmetry is considered as the constitutional, graph-theoretical, topological or combinatorial symmetry.

The two distinct kinds of symmetry are, of course, closely related. The equivalence of vertices in a constitutional formula is a necessary but not sufficient condition for the equivalence of the corresponding atoms in a spatial embedding of the real-life molecule.

3.2. Computer manipulation of constitutional formulas requires a special mathematical language. This is certainly the language of graph theory. For historical reasons, half a century ago graph theory was considered a part of topology. Perhaps this is the reason why chemists sometimes still refer to graph-theoretical properties of molecular models as to topological ones and use such terms as topological index and topological symmetry, see for example [Pre76], [Ran74], [HalK90], [LiuBM90a], [Ban94], [HuX94]. In fact, truly topological considerations appear in the chemical literature rather rarely, see for example [MerS89] (where finite topologies are used). However, topology is used in mathematical chemistry as a link between geometry and discrete mathematics, as discussed in [GutP86] and [Mez83].

3.3. By now, it is generally accepted that graph theory is an appropriate tool for mathematical modelling in chemistry. Books like [Bal76], [GutP86], [Tri92], [BonR91], [Rou90] provide a good introduction to both graph theory fundamentals and numerous applications in chemistry.

In chemistry, graphs serve as models for chemical objects and connections between them. The most important chemical graphs are molecular graphs (constitutional formulas: vertices represent atoms, edges bonds). Another important class of chemical graphs are reaction graphs (vertices represent molecular species, edges represent reactions, [Bal77], [KliZ91], [Bro94], [KvaP90]). In any case, the knowledge of the symmetry of a graph is significant or even crucial.

3.4. The symmetry of a graph is completely described in terms of its automorphism group. In turn, an automorphism group is a particular case of a permutation group, and the latter notion is less popular in chemical literature. Gutman and Polansky [GutP86] give a brief and very bright introduction to the subject, freely using the notion of a permutation group, but not defining it rigorously. Each of the references [BroGW83], [Hin79], [UgiDKM84], and [Fuj91] introduces some new area of application of group theory to chemistry. In the present series of papers, we intend to introduce to mathematical chemistry the ideas, methods and algorithms which are already commonly used in algebraic combinatorics. In particular, this initial paper of the series has as its main subject a combinatorial approach to the notion of 2-orbits of permutation groups, especially of automorphism groups of graphs. We start with briefly mentioning several areas of mathematical chemistry and chemical information where the use of combinatorial symmetry is absolutely necessary.

3.5. Analytical and constructive enumeration of chemical combinatorial objects (i.e. isomer generation) are classical (and the earliest) applications of permutation groups starting from A. Cayley [Cay875], A.C. Lunn and J.K. Senior [LunS29], J.H. Redfield [Red27] and G. Polya [Pol37]. For a detailed discussion of this class of problems see the chapter "Chemical Graphs" in the book [BigLW76]. Exhaustive graph enumeration has been important for many years in computer-assisted structure elucidation [Smi77], [Gra86], [KerLM90], it recently became urgent again in the explosive growth of fullerene chemistry [BabKS93], [KleL94]. Recent developments related to the use of so-called Burnside techniques in analytical enumeration are found in [Ker91], [Fuj91], [Llo92], see also the brief essay in Section 3.1 of [FarKM94]. Modern techniques for constructive enumeration can be learned from [BroM74], [CorM78], [Far78], [LamT89]. Applications to the generation of molecular graphs are presented in [GruKL92], [Mol94].

3.6. The graph isomorphism problem is certainly the central link between algebraic combinatorics and mathematical chemistry. Every chemist will many times solve such a problem "in mind" whenever it is necessary to identify or to distinguish two given compounds represented by their constitutional formulas. The huge number of known compounds necessitates efficient coding/decoding procedures ("nomenclature") in order to store and retrieve them by computer in large databases [BurMW94]. Finding a fast (polynomial-time) graph isomorphism algorithm was a challenging task with which a large number of scientists were (and are still) concerned. Like during an epidemic more and more people were seized with this challenge, reports on some progress attracted a new crowd of researchers. Eventually, the situation was characterised as "the graph isomorphism disease" in [ReaC77], [Gat79]. There and in [ZemKT82], [Bab81], [Hof82], [ButL85] one can find discussions of many facets of the problem and detailed classifications of different approaches to its solution. Discussions of the problem through the eyes of chemists are found for example in [BonMB85], [Gra86], [LiuK91].

For practically comparing graphs rigorous and heuristic methods can coexist. It is convenient to find rather frequently the answer "no" in isomorphism testing by means of a very simple and fast heuristic procedure. Then for a small number of structures which are most suspect of being isomorphic to a given one, the final answer will be achieved by a slower subroutine which is known to always give the correct answer.

From a theoretical point of view the most important achievement is that isomorphism of graphs of bounded valencies can be tested in polynomial time [Luk82]. This result was derived by using exhaustively group-theoretical methods. However, attempts to exploit this result in a practically helpful algorithm, e.g. [FurSS83], are not yet sufficiently successful.

3.7. The graph symmetry problem (i.e. the graph automorphism problem) in its most explicit form is encountered everywhere in the manipulation of chemical structures by hand or by computer. The questions of which atoms, bonds, pairs of atoms, etc., are equivalent in a structure have to be answered in order not to duplicate efforts. The answers to these questions, namely the partitions of the respective objects into equivalence classes, can be obtained more or less reliably using simple heuristic algorithms. Many such algorithms exist, most of them are concerned only with the partition of the atoms, the so-called *automorphism partition*. In other words, they try to find the *orbits* (*1-orbits* more exactly). The description of the 1-orbits is one of the oldest problems in mathematical chemistry. The classical paper [Mor65] by H. L. Morgan is considered as the starting point of the story. Almost at the same time the notion of canonical ordering of a graph was introduced by J. F. Nagle in [Nag66].

Starting with Morgan a tremendous amount of work was devoted to the problem of finding the automorphism partition of a graph. It is known that in terms of computational complexity this problem is equivalent to the isomorphism problem, which means that one can solve both of them simultaneously with about the same effort.

3.8. In Morgan's procedure initially all vertices are indistinguishable, i.e. they all belong to a single equivalence class. To indicate this fact, all vertices are equally weighted by assigning to each of them the attribute (weight) 1. In the following process weights of vertices are changed step by step. In each step, every vertex gets a new weight which is the sum of the weights of its neighbors. Vertices of the same weight form a new equivalence class. Unless the graph is regular this procedure will produce a sequence of partitions of the vertex set. It stops when at a new step no refinement of the current partition is achieved. The final partition is called a *stable partition.*

There are numerous generalizations and improvements of Morgan's procedure. To obtain a first impression the reader is referred to the survey [BalMB85]. A detailed discussion of different stabilization procedures will be presented in our forthcoming publications. In spite of several serious attempts to find more effective versions of the stabilization procedure, see e.g. [WipD74], [MekBB85], there is still no polynomial-time stabilization procedure which applied to an arbitrary input graph Γ gives as output the correct automorphic partition of Γ. Moreover, recent results in [CaiFI92] have destroyed the hope to obtain polynomial-time procedures when using so-called deep stabilization with bounded depth (see [Wei76] for definitions).

On the other hand, numerous heuristical stabilization procedures are rather quick and rather successful on certain classes of graphs. Adequate descriptions of such classes of graphs as, for instance in [Tin91], can create a more rigorous background for a restricted use of stabilization procedures.

3.9. One of the disadvantages of Morgan's and similar approaches is that these methods will not give any non-trivial partition of the vertex set of a regular graph (even not in the case when $Aut(\Gamma)$ is the trivial group, for details see [BalMB85]). To our knowledge Weisfeiler and Leman were the first to consider the more general problem of finding the 2-orbits of a graph, that is the partition of pairs of vertices into equivalence classes. Let Ω be the vertex set of a graph Γ and $G = Aut(\Gamma)$. Two pairs of vertices (x, y) and (u, v) are considered as equivalent if there is an automorphism $g \in G$ which maps x onto u and y onto v. Each maximal set of equivalent pairs of vertices is called a 2-*orbit* of G on Ω^2. The set of all 2-orbits is denoted by 2-$orb(G, \Omega)$, its construction is straightforward once the automorphism group is given. In this setting the automorphism partition of a graph is a byproduct of the determination of the 2-orbits: the 1-orbit for atom a is simply the 2-orbit of the pair (a, a), and this fact implies the partition of the vertex set of a regular graph.

From the algorithmic point of view, the paper [WeiL68] was based on ideas similar to Morgan's approach, i.e. on the use of an iterative stabilization procedure. The crucial advantage of the new approach was a systematic application of algebraic tools. Unfortunately, though the Weisfeiler–Leman procedure in many cases yields the set 2-$orb(G, \Omega)$ correctly, there are examples where this procedure fails. Such examples can be found for example in [Mat78] where a list of "difficult" highly symmetric graphs for testing isomorphism perception algorithms was given.

More or less the same as Weisfeiler–Leman's approach was independently elaborated by one of us and his coworkers in [HinT77], however, without explicitly using the group-theoretical notion of 2-orbits. The approach itself (as part of the theory of coherent algebras) is now rather familiar to the experts in algebraic combinatorics and discrete mathematics (see e.g. [KuzA85], [Hig87], [Fri89]), however, a careful investigation of its abilities is still lacking.

From the fact that Weisfeiler and Leman made reference to [Mor65] and from some additional remarks in their paper (as well as from [Ade95]) it is evident that their interest in the topic came from chemistry. However, during twenty years their ideas were completely unknown in mathematical chemistry.

3.10. While these approaches due to mathematicians were performed on a rather high mathematical level, chemists went their own ways. In a series of papers M. Uchino perhaps was the first in the chemical literature who used matrix multiplication for obtaining the automorphism partition [Uch80], [Uch82]. He exploited matrices of open walks and distance matrices, both produced from the adjacency matrix of a molecular graph. In the paper [CarSV85], the problem of classifying atom pairs was approached using simple graph invariants such as the color of atoms and their graph-theoretical distance. The reader will find in the literature also several publications where operations on matrices were used for similar goals (e.g. [Ber87], [Bal90], [LiuBM90a]).

Finally in 1989, two of us again independently realized the necessity of having a method for the partition of atom pairs, and produced a heuristic yet rather successful computer program for that purpose by simple reasoning without using any mathematical machinery [RueR90b], [RueR91a], [RueR91b]. This approach is very close to the two approaches mentioned in 3.9 with one distinction: a certain desymmetrization step (see 6.14) is not involved in the procedure.

However, all heuristic algorithms fail for some classes of more or less nasty graphs, and in most cases the limitations are not exactly known.

3.11. In the foregoing paragraphs we mentioned the three main computational problems of algebraic combinatorics: constructive enumeration of combinatorial objects, testing isomorphism of graphs and finding the automorphism group of a graph. Obviously, these problems are intimately related. Generation of isomers requires both symmetry recognition and graph isomorphism testing in order to avoid multiple construction of the same isomer. Testing two graphs for isomorphism is equivalent to looking for automorphisms of their disjoint union graph [ReaC77], [Mat79]. Conversely, finding the automorphism group of a graph can be considered as a special graph isomorphism problem: find all isomorphisms of the graph with itself.

The solutions to the above problems are more or less conveniently obtained once the graph's automorphism group $Aut(\Gamma)$ is known, as will be shown in the following sections. So it all boils down to the question of how to obtain this group. Here the use of strong generating systems of $Aut(\Gamma)$ (see Section 4) is of great advantage. There are a few well-known program implementations of backtracking algorithms for the computation of $Aut(\Gamma)$. Three of them, elaborated by J. S. Leon (see [Leo84]), by B. D. McKay (see [McK90]) and by I. A. Faradžev ([FarK91], [FarKM94]) are regarded as reasonably fast and efficient.

The modern approach to the solution of all these problems is based on common ideas, roughly speaking its main features look as follows:

> Graphs (and other combinatorial objects) are represented by means of matrices (adjacency matrix, incidence matrix, etc.). Matrices are encoded as words over some finite alphabet. All possible code words can be ordered lexicographically.
>
> In every class of isomorphic graphs, one graph with extremal value of its code word (for example with maximal value) is selected. This code word is called *canonical*, the graph which is described by the canonical code word is the *canonical representative* of its isomorphism class. To enumerate graphs means to find all different canonical code words. To test if two graphs are isomorphic or not means to compare the code words of their canonical representatives. To find the automorphism group means to find all permutations of the vertices of the graph which preserve the extremal value of the canonical code word.
>
> For constructive enumeration decision trees (search trees) are used in order to control the enumeration process and in order to reduce the total time needed for solving the enumeration problem. Special predicates are defined on the interior nodes of the decision tree. If in the course of the process a predicate on some interior node turns out to be false, then consideration of the descendants of this node can be dropped (see e.g. [Far78]). For testing graph isomorphism or for computing automorphism groups the decision tree is arranged via the so-called iterative classification where sequences of easily computable local invariants of vertices are systematically used to distinguish non-equivalent vertices ([FarKM94]).
>
> In all cases group theoretical information is permanently considered, collected and used. For example, when computing the automorphism group of a graph (see Section 4), the search tree controls a backtracking procedure for finding a strong generating set of the group. To select new permutations for this set, at every step of the algorithm the subgroup generated by the currently stored automorphisms and the cosets of this subgroup are considered. Using this strategy, considerable parts of the search tree can be excluded from further processing.

3.12. Many of the above ideas were independently developed in mathematics and in chemistry. For example, an algorithm for graph canonization was introduced in [ArlZUF74], and in chemical literature such an algorithm was proposed for the first time by M. Randić in [Ran74], see also [RanBW81]. In the paper [Tri86] a symbol manipulation system for computations with permutation groups is presented on a rather high level. In [UgiB-S93] effective procedures for economical storage and fast generation of permutations and their practical implementations are used.

However, the level of "group-theoretical literacy" involved in parts of mathematical chemistry still remains rather low. Up to date still a lot of heuristic algorithms for the solution of the above-mentioned problems (see e.g. [BieB92]) are elaborated and published, not only without rigorous theoretical background but also without any reference or comparison to algorithms and programs previously described. Sometimes even most experienced experts in mathematical chemistry are not using all the options, provided by the modern computational group theory. For example, the algorithm presented in [RazBM93] requires more than 82h of CPU time for computing the automorphism group of a certain "complex" 16-vertex graph (in fact, this graph is not even regular). An improved version of the algorithm described by one of the authors (see [Bal94a]) requires only 1 min 29 sec for processing the same graph. However, using the modern techniques briefly mentioned above should allow to reach the result significantly (at least 100 times) faster. The same author informs us in [Bal94b] that his algorithm will produce a complete list of all automorphisms of the input graph. For instance, generating and listing all 1036800 automorphisms of a certain edge-weighted 12-vertex graph (the automorphism group of which is the wreath product $S_2 \wr S_6$, see 4.30 for definition) needed 37.5 min of CPU time. This graph was processed by one of us using the computer package COCO on an IBM personal computer (see [FarK91], [FarKM94]) needing CPU time of 0.66 sec. The reason for this speed-up may be found in the fact that COCO uses a strong generating set for describing the automorphism group. In the case of $S_2 \wr S_6$ there exists a strong generating set of 11 elements only, which is enough for storing and providing access to the whole group. For more details concerning group-theoretical notions used here see 4.21.

We hope that this and forthcoming papers in our series will help to overcome the still existing disbalance between the actual abilities of algebraic combinatorics and its current very limited application in mathematical chemistry.

3.13. A detailed account of all illustrations, examples and facets of combinatorial symmetry goes far beyond the bounds of this paper. We shall restrict ourselves to the areas familiar to us and to results closely related to our taste and/or experience. The paper [UgiB-S93] containing 226 references is strongly recommended for a survey. It is written on the base of an algebraic model for the logical structure of constitutional chemistry which was suggested by J. Dugundji and I. Ugi [DugU73], [UgiS-W93].

In what follows our main attention is directed towards the problem of finding the 2-orbits and, as a byproduct, the 1-orbits of the automorphism group of a graph.

Generally, scientists are not only interested in objects, but also in relations between objects, and this is the reason why graphs are ubiquitous in science. Thus, chemists do not consider atoms as such, but atoms in the context of a molecule. Moreover, they are not fully content with molecules, but care about reactions (relations between molecules) or even reaction networks (relations between reactions). In other words they consider and classify pairs of objects. Therefore it is both very natural and important to obtain the 2-orbits of automorphism groups. For the remainder of this paper we shall concentrate on a narrower subject, the description of the 2-orbits of the automorphism groups of molecular graphs (2-orbits for reaction graphs, neglected here, are dealt with in [Bal77], [RanK-B87], [KliZ91], [KliTZ91], [BonR92], [JonL83], [Bro94], [LloJ98]).

3.14. There are several more reasons for taking care of 2-orbits of molecular graphs (pairs of atoms), a few are listed here:

(1) Finding all paths through a molecule is often required. A path represents a certain relation between its first and last atom, in fact, between all atoms involved. So if the paths between atoms x and y are already known, and if the pair of atoms (u, v) is known to be equivalent to the pair (x, y) by symmetry, then paths between u and v need not be traced: all their properties exactly correspond to those already known. This situation is encountered for example in chemical nomenclature, where the IUPAC rules for naming polycyclic compounds require finding all bridged cycles of maximum length in a molecule. A computer program written for automatically naming any polycycle is therefore supported by a symmetry perception program ([RueR90a] and [RueR90b]). Enumeration of all maximum length cycles without path-tracing (for a very special series of polycycles), based on the knowledge of the automorphism group, was demonstrated recently ([KliLP89], [KliLPZ92]).

Paths and numerical values associated to them are the basis of some of the most useful topological indices [KieH86]. Therefore calculation of such indices will profit from knowledge of the equivalence classes of atom pairs.

(2) Coupling phenomena in NMR spectroscopy reflect interactions within a pair of atoms in a molecule, see [Gue85] or any textbook of organic chemistry, e.g. [Vol87]. So the number of identical and distinct couplings found for a particular atom in a ^{13}C or ^{1}H NMR spectrum reflects the number of identical and distinct coupling partners for that atom. While the chemical shift information (number of 1-orbits) was used for computer-assisted structure elucidation, surprisingly the coupling information (number of 2-orbits) was not ([LiuBM90b], [Bal95a]).

(3) In synthesis planning by hand or by computer missing knowledge of the equivalences of bonds as well as of non-bonds in a molecule (pairs of atoms) will obviously result in duplication of efforts (see [ZefG87], [ZefGT88], [IhlG95]).

(4) Quantitative structure activity relationships (QSAR) are based on the dogma that compounds of similar structure exhibit similar biological activity. Molecular similarity can obviously be defined in various ways, [JohM90]. Sometimes it is expressed as numerical similarity of topological index values. Another approach is based on E. Fischer's lock-and-key idea: Since the drug receptor is a well defined arrangement of certain functional groups to be described in terms of geometrical distances, a potential drug will be characterized by a complementary arrangement of functional groups (hetero atoms) responsible for binding. Since geometrical distance information is usually not contained in large organic compound databases, in early work graph-theoretical distance information was used as a crude approximation. So similarity was described in terms of presence or absence of distinct atom pairs, such a pair being defined by the chemical nature of the atoms and by their graph-theoretical distance ([CarSV85]).

3.15. After all these foregoing considerations it is no surprise to see that sometimes chemists used notions which are very close to our notion of 2-orbits. For example in [ZlaE92] the problem of establishing a spatial model of a chemical compound is considered. The authors describe an iterative procedure which needs as input the adjacency matrix of a molecular graph Γ, some parameters of the desired spatial model of Γ and a description of the point group the model should have. The output are the 3D coordinates of the model produced. Implicitly, in the course of the iterations the procedure finds and reuses the 1-orbits, some of the 2-orbits and even some 3-orbits of $Aut(\Gamma)$ in order to find similar angles between the edges in the model of the molecular graph.

In the paper [StaTZ88] the authors use the notions of a base matrix and an equivalence matrix. According to their definition a base matrix is just a matrix which belongs to the centralizer algebra of the automorphism group of the given molecular graph, while the equivalence matrix completely describes the 2-orbits of the automorphism group.

3.16. Let Γ be a graph on the vertex set Ω and $G = Aut(\Gamma)$. We complete Section 3 stressing once more that we distinguish two different approaches to the description of $\mathit{2\text{-}orb}(G, \Omega)$: an empirical and a rigorous one.

Program implementations of the WL-stabilization process (see [BabCKP97]) as well as the algorithms TOPSYM and MATSYM ([RueR90b], [RueR91a]) serve in our opinion as successful examples of the empirical approach.

A rigorous approach to finding the 2-orbits of an automorphism group G is based on the knowledge of a set of generators for G. At first sight, this method may seem too roundabout: first we have to find G and then we have to study the induced action of this group on the pairs of vertices. However, our experience shows that this way is the only absolutely reliable one and that the time needed for this approach is rather acceptable for all graphs of say less than 1000 vertices. The corresponding algorithms and the results of tests with preliminary versions of computer programs are presented in [FarKM94]. A recent version of the program package has been described in [FarK91]. We believe that this rigorous approach (which was developed for processing "mathematical" graphs with high symmetry) will work most efficiently for chemical graphs if it is combined (in a clever portion) with a simple stabilization procedure used in a first phase of the processing. Modification and development of the existing program package for the use in mathematical chemistry is in our opinion the most important line of future activity.

4 Fundamentals of permutation group theory

Here we introduce a very elementary brief outline of the main notions from the theory of permutation groups. For more details we refer to [Wie64], [Big85] and [KliPR88].

4.1. Let G be a set (finite or infinite) and $*$ a *binary operation* on G. This means that for every $a, b \in G$ there exists a unique element $c = a * b \in G$ which is considered as the result of the application of $*$ to the ordered pair (a, b) of elements from G. G is called a *group* if

(G1) $a * (b * c) = (a * b) * c$ for all $a, b, c \in G$ (*associative law*);

(G2) there exists a *unique* element $e \in G$ such that $e * a = a * e = a$ for all $a \in G$ (*neutral element*);

(G3) for every element $a \in G$ there exists an *inverse* element $a^{-1} \in G$ such that $a^{-1} * a = a * a^{-1} = e$.[1]

For example, the set of non-zero rational numbers together with multiplication is a group. Likewise, the set of all integers including zero together with addition is a group. Accordingly, the sign $\cdot$ or $+$ may be used to denote a general group operation. Just as in the multiplication of numbers the sign $\cdot$ is often omitted. Thus, the result of the operation $\cdot$ between a and b may be written $a \cdot b$ or ab. The same type of capital letter (for example G) is used both for a set and for a group, since sometimes encountering a set together with an operation $*$ we do not know whether it is a group. If it is, then we also write $(G, *)$.

Let $|G|$ denote the cardinality of the set G. If G is finite, i.e. if $|G| = n$, then G is called a *finite group of order* n.

4.2. Let H be a subset of G, where $(G, \cdot)$ is a group. We shall say that $(H, \cdot)$ is a *subgroup* of $(G, \cdot)$ (denoted $H \leq G$) if $(H, \cdot)$ is a group with respect to the binary operation $\cdot$. In other words, H must be *closed* with respect to the group operation, i.e. $a \cdot b \in H$ for all $a, b \in H$, and the axioms (G1) - (G3) must be satisfied.

The set $H = \{\ldots - 8, -4, 0, 4, 8, \ldots\}$ together with addition is a subgroup of the second group mentioned above.

A *finite* subset H of G is a subgroup of $(G, \cdot)$, iff it is closed with respect to $\cdot$, i.e. (G1) - (G3) are then automatically satisfied ("iff" means "if and only if").

Let $H \leq G$. For $g \in G$ the set $Hg = \{hg : h \in H\}$ is called a *right coset* of G with respect to H. The notation Hg means: "Multiply" all elements of H by the particular element g from G. The set of all results h_1g, h_2g, $\ldots$ is the right coset Hg.

[1] This system of axioms contains redundancies, see e.g. [Hal59]. However, it is convenient for general use.

All elements of Hg are pairwise distinct. Moreover, two cosets Hg' and Hg'' are either disjoint or they are equal as sets. Hence, the group G can be *decomposed* into pairwise disjoint cosets $Hg_1, Hg_2, \ldots, Hg_m$ such that $G = Hg_1 \cup Hg_2 \cup \ldots \cup Hg_m$. If the number m of different cosets is finite then this number is called the *index* of the subgroup H in G. We use the notation $[G : H]$ for the index m of H.

EXAMPLE: Let G be the set of all integers together with the addition operation. Let $H = \{\ldots, -8, -4, 0, 4, 8, \ldots\}$. Take as g the number 1. Then $H + g = \{\ldots, -7, -3, 1, 5, 9, \ldots\}$. Now take as g' the number 2, to obtain $H + g' = \{\ldots, -6, -2, 2, 6, 10, \ldots\}$. Then $g'' = 3$ and $g''' = 4$ give $H + g'' = \{\ldots, -5, -1, 3, 7, 11, \ldots\}$ and $H + g''' = \{\ldots, -4, 0, 4, 8, 12, \ldots\} = H$. Obviously, these are the only such cosets, thus $[G : H] = 4$.

If $H \leq G$ and G is a finite group then

$$|G| = |H| \cdot [G : H].$$

This equality is often called *Lagrange's Theorem.*

We can also consider left cosets gH which are defined similarly. In general, the two decompositions of G into right and left cosets do not coincide.

In what follows our attention will be devoted to special representations of those groups which are called permutation groups.

4.3. Let Ω be a set. A *mapping* $f : \Omega \mapsto \Omega$ assigns to every element $x \in \Omega$ an image $y = x^f \in \Omega$. The mapping f is called

injective (mapping into), if $x \neq y \Rightarrow x^f \neq y^f$ holds for all $x, y \in \Omega$;

surjective (mapping onto), if for all $y \in \Omega$ there exists at least one $x \in \Omega$ such that $y = x^f$;

bijective (one-to-one mapping onto), if it is injective and surjective.

A bijective mapping from a finite set Ω onto itself is called a *permutation acting* on Ω.

For every mapping $f : \Omega \mapsto \Omega$ we can consider an *inverse correspondence* f^{-1} which to every $y \in \Omega$ associates a subset $y^{f^{-1}}$ of Ω where $x \in y^{f^{-1}} \Leftrightarrow y = x^f$. In general, $y^{f^{-1}}$ can contain more than one element, so that f^{-1} is not necessarily a mapping. The following proposition can be easily proved.

4.4. Proposition. *For a mapping f on a finite set Ω the following statements are equivalent:*

(a) f is injective;
(b) f is surjective;
(c) f is a permutation;
(d) the inverse correspondence f^{-1} to f is a mapping;

(e) the inverse correspondence f^{-1} to f is a permutation.

4.5. In what follows we shall consider permutations on a finite set Ω. In most applications considered later on, Ω will be the vertex set of a graph Γ. We shall use the notation $S(\Omega)$ for the set of all permutations acting on Ω. Let $f, g \in S(\Omega)$. The *product* $h = f \circ g$ (or simply fg) *of the permutations* f and g is the mapping $h : \Omega \mapsto \Omega$ for which $x^h = (x^f)^g$.

It can be easily proved that the product of two permutations is also a permutation. In this context the group operation $\circ$ is considered as a kind of "abstract" multiplication. This explains also the term "product" of f and g.

Consider the set $S(\Omega)$ together with the binary operation $\circ$. It turns out that $(S(\Omega), \circ)$ satisfies all axioms for a group. The neutral element in $S(\Omega)$ is the *identity* e defined by $x^e = x$ for all $x \in \Omega$, and for a permutation f of Ω the inverse element f^{-1} is the inverse permutation.
The group $S(\Omega)$ is called the *symmetric group* of the set Ω. If Ω consists of n elements then we will use also the notation S_n instead of $S(\Omega)$ (if the meaning of Ω is of no matter).

4.6. Here we list a few convenient ways for representing permutations.

In a *two-row table* associated with $g \in S(\Omega)$ all elements of Ω are presented in the first row and the corresponding images in the second row. For example

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ 3 & 7 & 5 & 8 & 2 & 4 & 1 & 6 \end{pmatrix}$$

is the permutation acting on $\{1, 2, 3, 4, 5, 6, 7, 8\}$ which sends 1 to 3, 2 to 7, 3 to 5, and so on.

The *diagram* $D(g)$ of g is a directed graph in which the vertices represent the elements of Ω and where an arc is drawn from each $x \in \Omega$ to its image x^g. Figure 4.1 shows the diagram of the permutation in the example above.

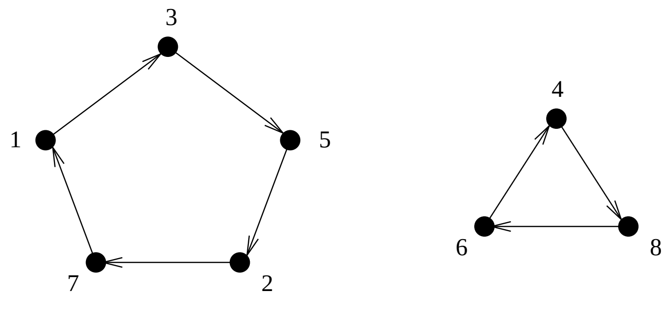


Figure 4.1.

Let $\Omega = \{1, 2, \ldots, n\}$ and let $M(g)$ be the adjacency matrix of the diagram $D(g)$, i.e.

$$M(g) = (m_{ij})_{1 \leq i,j \leq n}$$

where

$$m_{ij} = \begin{cases} 1 & \text{if} \quad j = i^g \\ 0 & \text{otherwise.} \end{cases}$$

The matrix $M(g)$ is a so-called *permutation matrix.* It contains exactly one entry equal to 1 in each row and in each column.

It can be easily seen that for every permutation $g \in S(\Omega)$ the diagram $D(g)$ is a union of disjoint *oriented cycles.* This enables us to encode every permutation by means of its *cyclic representation* (or equivalently, as we shall say, by its *decomposition into a product of disjoint cycles*). Thus, if $D(g)$ consists of l cycles of lengths $k_1, k_2, \ldots, k_l$ where $k_1 + k_2 + \ldots k_l = n$, then we shall write

$$g = (a_1, a_2, \ldots, a_{k_1})\,(b_1, b_2, \ldots, b_{k_2}) \ldots (u_1, u_2, \ldots, u_{k_l}).$$

Accordingly, the two-row representation of g is

$$g = \begin{pmatrix} a_1 & a_2 & \ldots & a_{k_1} & b_1 & b_2 & \ldots & b_{k_2} & \ldots & u_1 & u_2 & \ldots & u_{k_l} \\ a_2 & a_3 & \ldots & a_1 & b_2 & b_3 & \ldots & b_1 & \ldots & u_2 & u_3 & \ldots & u_1 \end{pmatrix}.$$

The cyclic representation of the permutation in the above example is (1, 3, 5, 2, 7) (4, 8, 6).

Usually cycles of length 1 are omitted. The notation of each cycle starts with its smallest number, cycles are arranged according to increasing first numbers. If these conventions are adopted then every permutation is represented by its unique *canonical cycle decomposition.*

4.7. EXAMPLE:
Let $n = 10$ and

$$g_1 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \end{pmatrix},$$

$$g_2 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\ 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 1 \end{pmatrix},$$

$$g_3 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\ 3 & 1 & 5 & 9 & 6 & 2 & 7 & 4 & 8 & 10 \end{pmatrix}.$$

Here, g_1 is the identity, g_2 is a cycle of length 10. We give a few different codes for g_3, the last of them is canonical. Also $M(g_3)$ is presented.

$$g_3 = (5, 6, 2, 1, 3)(7)(9, 8, 4)(10) = (7)(10)(8, 4, 9)(2, 1, 3, 5, 6) = (1, 3, 5, 6, 2)(4, 9, 8),$$

$$M(g_3) = \begin{pmatrix} 0&0&1&0&0&0&0&0&0&0 \\ 1&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&1&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&1&0 \\ 0&0&0&0&0&1&0&0&0&0 \\ 0&1&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&1&0&0&0&0 \\ 0&0&0&1&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&0&0&1 \end{pmatrix}.$$

4.8. Let $G \subset S(\Omega)$ be a subset of $S(\Omega)$ which is closed with respect to multiplication of permutations. Then according to 4.2 G is a group. In such a case G is called a *permutation group* acting on Ω. We shall use the notation (G, Ω) in order to stress that a permutation group is a pair "group, set", where the "group" consists of permutations which act on the "set".

The routine way to prove that a given set G of permutations is a group is to check that this set is closed with respect to multiplication.

4.9. Example:
Let $\Omega = \{1, 2, 3, 4\}$, and $G = \{g_1,\ g_2,\ g_3,\ g_4\}$ where

$$g_1 = e,\ g_2 = (1,2)(3,4),\ g_3 = (1,3)(2,4),\ g_4 = (1,4)(2,3).$$

Since $g_2 g_3 = g_3 g_2 = g_4,\ g_2 g_4 = g_4 g_2 = g_3,\ g_3 g_4 = g_4 g_3 = g_2,\ g_1^2 = g_2^2 = g_3^2 = g_4^2 = e$, the set G is closed with respect to multiplication. Hence (G, Ω) is a permutation group.

4.10. If G has many elements then it is practically impossible to check the group property by direct computations. In such a case the following general principle can be used instead. Let G consist of all permutations from $S(\Omega)$ which *preserve a certain property* of the elements of Ω. Then G is a permutation group. We do not give here a rigorous explanation of the term "property". [1] Instead, we restrict ourselves to the consideration of a few examples. Later on, this general principle will be reformulated in terms of graphs, which will be the most important case in our considerations.

4.11. Example:
Let $\Omega = \{1, 2, 3, 4\}$ and let G consist of all permutations from $S(\Omega)$ which preserve the partition $\{\{1, 2\}, \{3, 4\}\}$ of Ω (in other words: each $g \in G$ sends $\{1, 2\}$ onto itself or onto $\{3, 4\}$, and the same requirement is for $\{3, 4\}$). Then we can certainly claim (even without knowledge of all elements in G) that (G, Ω) is a permutation group. We suggest to the reader to check that

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

[1] This can be done in the language of m-ary relations, see e.g. [KalK72], [KliPR88].

4.12. EXAMPLE:
The following example may seem a little exotic. The property preserved here is a certain polynomial. Let $f(x_1, x_2, x_3) = x_1x_2^2 + x_2x_3^2 + x_3x_1^2$ and $\Omega = \{1, 2, 3\}$. For $g \in S(\Omega)$ define

$$f^g(x_1, x_2, x_3) = f(x_{1^g}, x_{2^g}, x_{3^g}).$$

For example, with $g = (1, 2)$ we have

$$f^g(x_1, x_2, x_3) = x_2x_1^2 + x_1x_3^2 + x_3x_2^2.$$

Let G be the set of permutations in $S(\Omega)$ which leave the polynomial $f(x_1, x_2, x_3)$ unchanged. Then again, (G, Ω) is a permutation group. We find $G = \{e,\ (1, 2, 3),\ (1, 3, 2)\}$.

4.13. Let (G, Ω) be a permutation group. Let
$X = \{x_1, x_2, \ldots, x_k\} \subset \Omega$,
$G_{x_1,\ldots,x_k} = \{g \in G \,:\, x_1^g = x_1, x_2^g = x_2, \ldots, x_k^g = x_k\,\}$,
$G_{\{x_1,\ldots,x_k\}} = \{g \in G \,:\, X^g = X\,\}$,
where $X^g = \{x_1^g, x_2^g, \ldots, x_k^g\,\}$. Then again it is easy to see that $G_{x_1,\ldots,x_k}$ and $G_{\{x_1,\ldots,x_k\}}$ are subgroups of G which are called the *pointwise stabilizer* of X in G and the *setwise stabilizer* of X in G, respectively. If $X = \{x\}$ is a 1-element subset of Ω then the notions of G_x and $G_{\{x\}}$ coincide and usually only the first notation is used.

For example, G_{x_1,x_2} is the set of all permutations that do not change the objects x_1 and x_2 while $G_{\{x_1,x_2\}}$ is the set of all permutations that fix the set of objects $\{x_1, x_2\}$, that is either do not change x_1 and x_2 or just interchange them.

4.14. Let (G, Ω) be a permutation group. We say that the elements $x, y \in \Omega$ belong to the same *orbit* of (G, Ω) if $y = x^g$ for a suitable $g \in G$. This means, an orbit is the set of all objects which are obtainable from one another by the actions of the permutations in G. Obviously, the set of all different orbits of (G, Ω) forms a partition of Ω. This means that different orbits have empty intersection and the union of all orbits is equal to Ω. The number of elements which belong to the orbit Orb, denoted by $|Orb|$, is called the *length* of Orb. A permutation group (G, Ω) is called *transitive* if Ω is its only orbit, otherwise it is called *intransitive*. Hence transitivity of (G, Ω) means that for every pair (x, y), $x, y \in \Omega$ there is a permutation $g \in G$ such that $y = x^g$.

All permutation groups considered in 4.9, 4.11 and 4.12 are transitive.

4.15. Proposition. *Let (G, Ω) be a permutation group. For $x \in \Omega$ let $Orb_G(x)$, or simply $Orb(x)$, be the orbit of (G, Ω) which contains x. Then*

$$|Orb(x)| = [G \,:\, G_x] = \frac{|G|}{|G_x|}.$$

Thus, in words, the number of elements in each orbit is a divisor of the group order.

Proof. To prove the proposition consider the partition of G into right cosets with respect to the stabilizer G_x of x. These cosets are in one-to-one correspondence with the elements of $Orb(x)$. The second equation holds due to Lagrange's Theorem. $\diamond$

4.16. EXAMPLE: Let

$\Omega = \{1, 2, 3, 4, 5\}$,
$g_1 = e, \;\; g_2 = (1, 2, 3), \;\; g_3 = (1, 3, 2)$,
$g_4 = (1, 2)(4, 5), \;\; g_5 = (1, 3)(4, 5), \;\; g_6 = (2, 3)(4, 5)$,
$G = \{g_1, g_2, g_3, g_4, g_5, g_6\}$.

We challenge the reader to prove that with this definition of G and Ω the pair (G, Ω) is indeed a permutation group. This group is intransitive with two orbits $X_1 = \{1, 2, 3\}$ and $X_2 = \{4, 5\}$. We have $G_1 = \{g_1, g_6\}$, such that $|X_1| = |Orb(1)| = [G : G_1] = 3$. Furthermore, $G_4 = \{g_1, g_2, g_3\}$ and $|X_2| = |Orb(4)| = [G : G_4] = 2$.

4.17. The set $\Omega^2 = \{(a, b) : a, b \in \Omega\}$ of all possible pairs of elements in Ω is called the *Cartesian square* of Ω. Every subset $R \subset \Omega^2$ is called a *binary relation* on Ω. For a binary relation R, let $R^t = \{(b, a) : (a, b) \in R\}$. A binary relation R is called *symmetric* if $R^t = R$; it is called *antireflexive* if $(a, a) \notin R$ for all $a \in \Omega$.

The Cartesian square can be imagined literally as a square matrix of $n \times n$ elements (if $|\Omega| = n$), and a binary relation as a scattering of 1's over this matrix which otherwise is occupied by zeros.

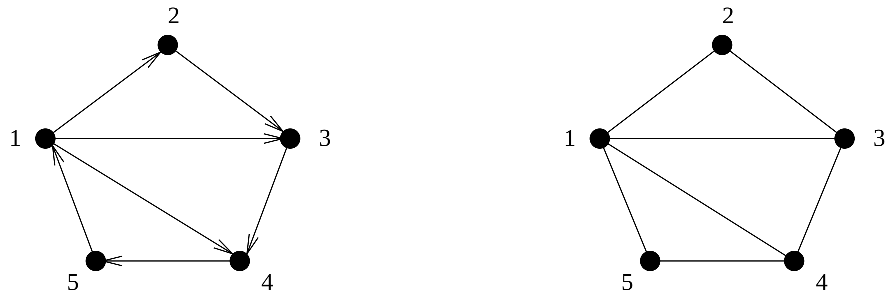


Figure 4.2.

A *directed graph* $\Gamma = (\Omega, R)$ is a pair which consists of a set Ω of *vertices* and of a set R of arcs where $R \subset \Omega^2$ is a binary relation on Ω. A graph Γ can be visualized by depicting its *diagram*. Vertices are usually visualized by small bold circles, arcs by arrows (see Figure 4.2). The graph Γ is called *undirected* if R is a symmetric relation. Each pair $\{(a, b), (b, a)\}$ of opposite arcs in an undirected graph Γ can be identified with the 2-element set $\{a, b\}$, which is called an *edge* of Γ. In this way, the edge set of an undirected graph is a subset of $\left\{{\Omega \atop 2}\right\}$, the set of all 2-element subsets of Ω. We shall denote this edge set by E. Usually, an edge is depicted on the diagram of Γ as a line without arrows.

4.18. EXAMPLE:
Let
$\Omega = \{1, 2, 3, 4, 5\}$,
$R = \{(1, 2), (1, 3), (1, 4), (2, 3), (3, 4), (4, 5), (5, 1)\}$,
$E = \{\{1, 2\}, \{1, 3\}, \{1, 4\}, \{2, 3\}, \{3, 4\}, \{4, 5\}, \{1, 5\}\}$.
The directed graph $\Gamma_1 = (\Omega, R)$ and the undirected graph $\Gamma_2 = (\Omega, E)$ are depicted in Figure 4.2.

4.19. Let $g \in S(\Omega)$. The action of g on Ω can be extended to an *induced action* on Ω^2 in the following manner: for $(a, b) \in \Omega^2$ we define $(a, b)^g = (a^g, b^g)$.

For $R \subset \Omega^2$ define $R^g = \{(a, b)^g : (a, b) \in R\}$. In general $R^g \neq R$. If $R^g = R$ then we call g an *automorphism* of the relation R. Hence, an automorphism of a graph Γ is a permutation of its vertex set which preserves its arc set. The automorphisms of an undirected graph $\Gamma = (\Omega, E)$ are exactly the automorphisms g of the underlying symmetric relation $R = R^t$.

Let $G = Aut(\Gamma)$ be the set of all automorphisms of a graph $\Gamma = (\Omega, R)$. Application of the general principle from 4.10 immediatly shows that (G, Ω) is a permutation group. *Automorphism groups of graphs* (especially of chemical graphs) will be the main subject of our planned series of papers.

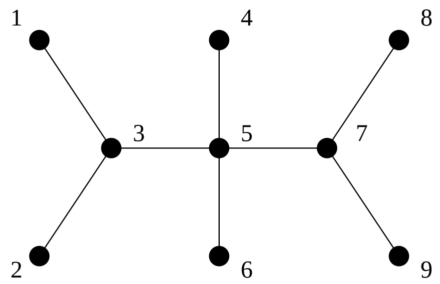


Figure 4.3.

4.20. EXAMPLE:
Let $\Omega = \{1, 2, 3, 4, 5, 6, 7, 8, 9\}$. Let Γ be the undirected graph with vertex set Ω which is depicted in Figure 4.3. Let $G = Aut(\Gamma)$. It can be easily found "visually" that (G, Ω) has the following orbits:

$$X_1 = \{1, 2, 8, 9\},\ X_2 = \{3, 7\},\ X_3 = \{4, 6\},\ X_4 = \{5\}.$$

We want to avoid listing all the automorphisms of Γ. Instead we restrict ourselves to finding the order $|G|$. Using a few times the formula in 4.15 we obtain:
$|G| = |Orb_G(1)| \cdot |G_1| = 4 \cdot |G_1|$,
$|G_1| = |Orb_{G_1}(8)| \cdot |G_{1,8}| = 2 \cdot |G_{1,8}|$,
$|G_{1,8}| = |Orb_{G_{1,8}}(4)| \cdot |G_{1,8,4}| = 2 \cdot |G_{1,8,4}|$,
$G_{1,8,4} = \{e\}$, hence $|G| = 4 \cdot 2 \cdot 2 \cdot 1 = 16$.

Note that $|Orb_{G_1}(8)|$ is the number of vertices in the orbit which contains vertex 8 in that subgroup of G which does not change vertex 1. "Visual" arguments were also used for finding the orbits of the subgroups of (G, Ω).

4.21. Let (G, Ω) be a permutation group with $g_1, g_2, \ldots, g_m \in G$ and let every permutation $g \in G$ be representable as a product $g_{i_1} \cdot g_{i_2} \cdot \ldots \cdot g_{i_k}$ where $i_1, i_2, \ldots, i_k \in \{1, 2, \ldots, m\}$. Then the set $\{g_1, g_2, \ldots, g_m\}$ is called a *generating set* of G. We say that G is *generated* by $g_1, g_2, \ldots, g_m$, and use the notation $G =< g_1, g_2, \ldots, g_m >$.

If, in particular, the group G is generated by a single permutation g then G is called a *cyclic group*.

Assume that $F = \{g_1, \ldots, g_m\} \subset G$ is a generating set for G and take an arbitrary $x \in \Omega$. Then, in general, there is no guarantee that G_x is generated by some subset of F. Therefore, it is sometimes very convenient to consider a special set F of generators for a permutation group (G, Ω), which in [Sim71], [Sim78] is called a *strong generating set with respect to some sequence* $(x_1, x_2, \ldots, x_k)$ *of different elements in* Ω. This sequence is called a *base* of the group if $G_{x_1,x_2,\ldots,x_k} = \{e\}$. A strong generating set F has the property that the stabilizer $G_{x_1,x_2,\ldots,x_l}$, $l \leq k$, of every initial subsequence of the sequence $(x_1, x_2, \ldots, x_k)$ is generated by a suitable subset of F.

The use of a strong generating set has many advantages. For example, it is easy to compute the order of (G, Ω), every permutation in (G, Ω) has a unique representation by strong generators, etc.

4.22. To have an example, let us turn back to the group G from 4.11. Let $g = (1, 3, 2, 4)$ and $h = (1, 3)(2, 4)$. Check that the products g, g^2, g^3, $g^4 = e$, h, gh, g^2h, g^3h are all the permutations in (G, Ω). All other products such as ghg, hgh etc. represent the same permutations. Hence $G =< g, h >$. Nevertheless, the set $\{g, h\}$ is not a strong generating set, since it is impossible to find a base as required for such a set.

4.23. Let us return to the permutation group (G, Ω) in paragraph 4.20. Let $x_1 = 1, x_2 = 8, x_3 = 4$. As shown in 4.20, $G_{1,8,4} = \{e\}$. Hence, the sequence 1, 8, 4 is a base of (G, Ω). Let $g_1 = (1, 2)$, $g_2 = (1, 8)(2, 9)(3, 7)$, $g_3 = (8, 9)$, $g_4 = (4, 6)$. Then

$$G_{1,8,4} = \{e\},\ G_{1,8} =< g_4 >,\ G_1 =< g_3, g_4 >,\ G =< g_1, g_2, g_3, g_4 >,$$

so that $\{g_1, g_2, g_3, g_4\}$ is a strong generating set for (G, Ω). [1]

4.24. In general, the problem of describing the automorphism group of a given graph $\Gamma = (\Omega, A)$ with $n = |\Omega|$ can be solved by *exhaustive search*. Roughly speaking, at the beginning of the search each of the $n!$ permutations in $S(\Omega)$ will be considered as a possible

[1] Sometimes it is convenient to consider a special kind of a strong generating set which satisfies additional requirements. This leads to the definition of a *standard system of generators* with respect to a given base (see [ZaiKF80] for a rigorous definition). This kind of generating set is quite useful in computer recognition of graph symmetries.

automorphism, however, in the course of the procedure only correct "candidates" will be selected. The history of the graph isomorphism problem, which is intimately connected to the problem of finding the automorphism groups of graphs, is also a history of the permanent struggle against the disadvantages of an exhaustive search. This question will be considered in more detail in forthcoming publications of our planned series.

4.25. The traditional approach to the description of the symmetry of chemical compounds is based on the use of transformation groups of the 2- or 3-dimensional space. This means that certain automorphisms of molecular graphs are interpreted as the action of rotations or reflections of space, restricted to a finite set of points which represent the atoms in the structural formula of a molecule. In many cases, only some automorphisms can be described in such a manner, so we can distinguish between *"spatial"* (or *"geometrical"*) and *"combinatorial"* symmetry of molecular graphs. Note also that for plane molecules considered in 3D-space it can happen that the same permutation corresponds to a few different geometrical symmetries (cf. [KliPR88], Section 1.6)[1].

Let us consider the graph Γ from 4.20 as a simple example. Let us associate with the vertices of Γ the set of points in the plane as depicted in Figure 4.3. Then only 4 of the 16 automorphisms of Γ will obtain a natural geometric interpretation, these are (in the notation of 4.23): $e,\ g_2,\ g_1g_4$ and $g_1g_2g_4$. The set $H = \{e,\ g_2,\ g_1g_4,\ g_1g_2g_4\,\}$ forms a subgroup of $Aut(\Gamma)$ which can be considered as "the geometrical 2D-subgroup" of the group $Aut(\Gamma)$.

Sometimes a combination of geometrical and combinatorial reasoning can be rather helpful for elaborating the automorphism group of a graph by hand.

4.26. EXAMPLE:
The graph Γ depicted in Figure 4.4 is an abstract picture of the molecule known as *"cuneane"*. It is a regular graph of degree 3. We can find its automorphism group $Aut(\Gamma)$ using a standard backtracking technique, see e.g. [McK81] or [KliPR88]. In order to avoid long routine computations let us start using the rather evident information about the "geometrical part" of $Aut(\Gamma)$. That is, let us consider the permutations $g_1 = (1,8)(2,3)(6,7)$ and $g_2 = (2,7)(3,6)(4,5)$ in $S(\Omega)$ where $\Omega = \{1,2,3,4,5,6,7,8\}$. These permutations represent two different reflections in 3D-space which are symmetries of the spatial model of cuneane, while g_1g_2 is a rotation around the axis cutting edges $(1,8)$ and $(4,5)$. It is evident that $H = \{e,\ g_1,\ g_2,\ g_1g_2\,\}$ is closed with respect to multiplication. Hence, H is the "geometrical subgroup" of $Aut(\Gamma)$. The sets

$$X_1 = \{1,8\},\ X_2 = \{2,3,6,7\},\ X_3 = \{4,5\}$$

are the orbits of the permutation group (H,Ω). Now we shall describe the whole automorphism group $G = Aut(\Gamma)$. Since H is a subgroup of G, the partition resulting from

[1]The notion of a permutation group can be generalized. Let G be an arbitrary group (sometimes we speak of an "abstract" group if the nature of its elements is of no matter). For a suitable finite set Ω a permutation group (G,Ω) can be defined by an isomorphism of G onto some subgroup of the symmetric group $S(\Omega)$. Let us consider homomorphisms into $S(\Omega)$ instead of isomorphisms (for an explanation of both notions see [Ker91] or [Hal59]). Then we obtain a more general notion of the action of G on the set Ω. In this way every permutation group G can be regarded as a *faithful* action on Ω.

H, $X_1 \cup X_2 \cup X_3$, is either finer than or identical to the true partition resulting from G, the automorphism partition. Now let us look at the structure and construct a very coarse partition of vertices by inspection. It is easily seen that vertices 1 and 8 play a role different from that of vertices 4 and 5 or the remaining vertices (1, 8 are the only ones not involved in the two triangles, 4, 5 are the only ones connected by an edge between different triangles). Therefore, the automorphism partition is equal to or finer than the one with the three classes $\{1, 8\}$, $\{4, 5\}$ and $\{2, 3, 6, 7\}$. Combining this observation with the previous one about the orbits of H, we get finally that the orbits of H are identical with the orbits of G. However, it is still possible that G is larger than H.

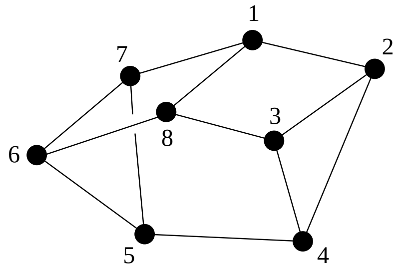


Figure 4.4.

Now in order to describe the whole automorphism group, let us first find a base of this group. Let us fix an arbitrary representative in each orbit, say $1 \in X_1$, $2 \in X_2$ and $4 \in X_3$, and consider the subgroup $G_{1,2,4}$. It is easily seen that every vertex of cuneane is uniquely determined by its adjacency to the vertices 1, 2 and 4, hence $G_{1,2,4} = \{e\}$. Vertices 4 and 5 can be distinguished by their respective adjacency to 1 and 2, that is an automorphism which fixes 1 and 2 will never move 4 to 5. So 1, 2 is also a base, $G_{1,2} = \{e\}$, in fact, being shorter it is a preferable one. Now the order of the automorphism group can be calculated:

$$|G| = |Orb_G(2)| \cdot |G_2| = 4 \cdot |G_2|,$$

$$|G_2| = |Orb_{G_2}(1)| \cdot |G_{2,1}| = 1 \cdot |G_{2,1}| = |G_{2,1}| = 1,$$

so that $|G| = 4$ and therefore $G = H$.

We have proved that in this particular case every "combinatorial" automorphism of the graph Γ has a geometrical meaning. As we know this is not true in general.

4.27. In chemistry, as well as in other areas of applied graph theory, graphs are used as models for structured sets (sets of atoms in molecules or of some other kind of items), the structure being defined by relations between the elements. As we have pointed out already, the automorphism group of such sets describes the symmetries of the structure, the geometrical as well as the purely combinatorial symmetries. Also some additional features of the structure can be reflected by corresponding features of the automorphism group. Thus, if a graph is made up of independent subgraphs, its automorphism group will be some "combination" of the automorphism groups of the subgraphs.

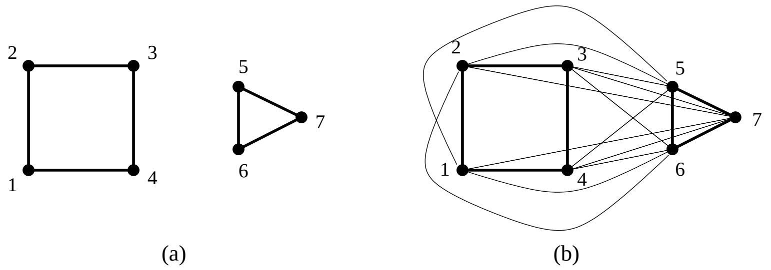


Figure 4.5.

Consider Figure 4.5a where a graph Γ is depicted which consists of a triangle and a square. Clearly, since a triangle and a square is a pair of non-isomorphic graphs, no automorphism of Γ can move a vertex of the triangle onto the square, and vice versa. Hence each $g \in Aut(\Gamma)$ is composed of some permutation g' of the vertex set $\{1, 2, 3, 4\}$ and some permutation g'' of the vertex set $\{5, 6, 7\}$. Therefore, if we know the action of g' on $\{1, 2, 3, 4\}$ and the action of g'' on $\{5, 6, 7\}$, we can describe the action of g as

$$x^g = \begin{cases} x^{g'} & \text{if} \quad x \in \{1, 2, 3, 4\} \\ x^{g''} & \text{if} \quad x \in \{5, 6, 7\}. \end{cases}$$

Now, assume that we have two permutation groups (G', Ω') and (G'', Ω'') acting on the disjoint sets Ω' and Ω'', respectively. Define

$$\begin{aligned} \Omega &= \Omega' \cup \Omega'' \\ G &= \{\, g' + g'' \;:\; g' \in G', g'' \in G'' \,\} \end{aligned}$$

where

$$x^{g'+g''} = \begin{cases} x^{g'} & \text{if} \quad x \in \Omega' \\ x^{g''} & \text{if} \quad x \in \Omega''. \end{cases}$$

The group G is called the *direct sum* of G' and G'' and is denoted by $G' + G''$. [1]

As an example, denote the triangle in Figure 4.5a by C_3, the square by C_4. Let $G' = Aut(C_3)$ and $G'' = Aut(C_4)$. In Γ all vertices of C_3 are equally related to all vertices of C_4. This fact is reflected by the structure of $Aut(\Gamma)$, namely

$$Aut(\Gamma) = Aut(C_3) + Aut(C_4).$$

We will determine $Aut(C_n)$ for undirected cycles C_n of arbitrary length n in subsection 4.32. It will turn out that the order of $Aut(C_n)$ is $2n$. Then, knowing these groups for $n = 3$ and $n = 4$, we are able to write down the 48 automorphisms of Γ immediately.

[1] The operation of *direct sum* is defined here as an operation over permutation groups. Note that in group theory one usually considers the operation of *direct product* of groups. Here we as a rule avoid the use of this term.

4.28. Proposition. *Let* $\Gamma = (\Omega, R)$, $\Gamma' = (\Omega', R')$ *be two graphs with disjoint vertex sets. Let*

$$\Gamma \cup \Gamma' = (\Omega \cup \Omega', R \cup R')$$

be the disjoint union of the graphs Γ *and* Γ'. *If* Γ *and* Γ' *are non-isomorphic and both connected, then*

$$Aut(\Gamma \cup \Gamma') = Aut(\Gamma) + Aut(\Gamma).$$

The proof of this proposition is straightforward and uses the same arguments as we used in the particular case of the example in 4.27. An automorphism which maps a vertex x of Γ onto a vertex x' of Γ' has to map the connected component of x (which is Γ itself) onto the connected component of x' (which is Γ'). Since Γ and Γ' are supposed to be non-isomorphic no such automorphism can exist. On the other hand, any automorphism of Γ can be combined with any automorphism of Γ' to give an automorphism of the disjoint union.

4.29. The notion of the direct sum of groups can be useful also for the description of the automorphism group of a connected graph Γ. Let $\Gamma = (\Omega_1, R_1)$ and $\Gamma_2 = (\Omega_2, R_2)$ be two graphs with $\Omega_1 \cap \Omega_2 = \emptyset$. The *disjoint sum* of these two graphs is the graph which consists of Γ and Γ' and all edges with one end in Ω_1 and the other end in Ω_2. We denote it by $\Gamma + \Gamma'$. More precicely,

$$\Gamma + \Gamma' = (\Omega_1 \cup \Omega_2, R_1 \cup R_2 \cup R_3)$$

where $R_3 = \Omega_1 \times \Omega_2 \cup \Omega_2 \times \Omega_1$. To have an example, consider Figure 4.5b which shows the disjoint sum of C_4 and C_3.

Let us show that $Aut(C_4+C_3) = Aut(C_4)+Aut(C_3)$. In spite of the fact that this equality may be regarded as rather obvious we prefer to give a succinct proof for it.

Comparing valencies of vertices in $C_4 + C_3$ we see that each automorphism g of $C_4 + C_3$ preserves the subsets $\Omega_1 = \{1, 2, 3, 4\}$ and $\Omega_2 = \{5, 6, 7\}$. Thus each automorphism belongs to the direct product $S_4 \times S_3$ of symmetric groups acting on Ω_1 and Ω_2, respectively. In the next step we observe that g even preserves the subgraphs of $C_4 + C_3$ generated by Ω_1 and by Ω_2. Therefore, $g \in Aut(C_4) + Aut(C_3)$. Finally, we check that $Aut(C_4) + Aut(C_3)$ is a subgroup of $Aut(C_4 + C_3)$. Now this implies

$$Aut(C_4 + C_3) = Aut(C_4) + Aut(C_3).$$

Arguments which are presented here to deal with a rather simple situation will be considered in more general context in Section 7.

4.30. A situation similar to the one in Figure 4.5 is shown in Figure 4.6. Here the graph $\Gamma = (\Omega, E)$ on the left side is depicted incompletely by only outlining some of its parts. The dashed areas are meant to contain isomorphic connected graphs Γ_1, Γ_2, Γ_3 and Γ_4, all isomorphic to some graph Γ_{inn} (the notation is deduced from the word "inner"), where

$\Gamma_i = (\Omega_i, E_i)$ such that $\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3 \cup \Omega_4$. The bold edges connecting Γ_i and Γ_j indicate the fact that each vertex in Γ_i is connected by an edge to each vertex in Γ_j. In this way the Γ_i's and the bold edges define a simplified picture of Γ which is called the *outer graph*, while the Γ_i's are called *inner graphs*. In our example the outer graph Γ_{out} has vertex set $\Omega_{out} = \{1, 2, 3, 4\}$ and edge set $E_{out} = \{\,\{1, 2\}, \{1, 4\}, \{2, 3\}, \{3, 4\}\}$. For the inner graphs the reader may take isomorphic copies of any graph Γ_{inn} he likes in order to complete his own individual example.

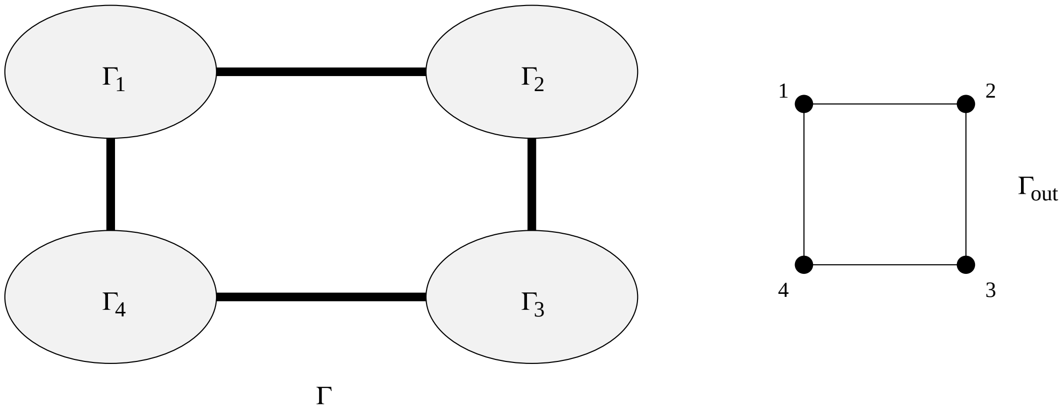


Figure 4.6.

Now, assume that we know the automorphism groups $Aut(\Gamma_i)$ of the inner graphs Γ_i. Since the Γ_i's are isomorphic, their automorphism groups are isomorphic, too, hence we shall denote them by $Aut(\Gamma_{inn})$, independently of i. Then to every $g \in (Aut(\Gamma_{inn}), \Omega_i)$ there is a corresponding automorphism $\bar{g}$ of Γ defined by

$$x^{\bar{g}} = \begin{cases} x^g & \text{if} \quad x \in \Omega_i \\ x & \text{if} \quad x \in \Omega_j,\ j \neq i. \end{cases}$$

Let G'' be the group of all automorphisms of this kind which we can get from the group $Aut(\Gamma_{inn})$. Note that, while all groups $Aut(\Gamma_i)$, $i = 1, 2, 3, 4$, are isomorphic to $Aut(\Gamma_{inn})$ as permutation groups, they act on different sets Ω_i.

Since all the inner graphs Γ_i are isomorphic, as we assume, there are still more automorphisms of Γ, which are to be described in a more complicated way. Assume that $\Omega_i = \{\,\omega_{i,1}, \omega_{i,2}, \ldots, \omega_{i,k}\,\}$ and that for arbitrary i, j the mapping $\phi_{ij} : \Omega_i \longrightarrow \Omega_j$ defined by

$$(\omega_{i,s})^{\phi_{ij}} = \omega_{j,s},\ 1 \leq s \leq k,$$

is an isomorphism from Γ_i onto Γ_j. (We can always find orderings of the sets Ω_i which fulfill this assumption.)

Now, assume in addition that we also know the automorphism group of the outer graph Γ_{out}. Let $h \in Aut(\Gamma_{out})$. We are prepared now to define a second kind of automorphism for Γ, namely the mapping g defined by

$$(\omega_{i,s})^g = \omega_{i^h,s},\ 1 \leq i \leq n_{out},\ 1 \leq s \leq k,$$

where n_{out} is the number of vertices in the outer graph ($n_{out} = 4$ in our example). This automorphism of Γ moves the inner graphs as a whole according to the connections in the outer graph. Let G' be the group of automorphisms which we get in this way. Clearly, G' is isomorphic to $Aut(\Gamma_{out})$.

Now consider the following procedure for constructing a permutation of the whole vertex set of Γ. First choose $h \in Aut(\Gamma_{out})$ and permute the inner graphs Γ_i according to h. Then apply permutations $g_i \in Aut(\Gamma_i)$ to the vertex sets of the inner graphs Γ_i, $1 \leq i \leq n_{out}$. The result is an automorphism of Γ. Let G be the group of automorphisms which are constructed in this way. Each element of G is a combination of some element in G' with some elements in G''. For this reason, G is also considered as a certain product of G' and G''. It is called the *wreath product* of G' and G'' and denoted by

$$G = G' \wr G''.$$

It follows from our description that

$$|G| = |G'| \cdot |G''|^{n_{out}}.$$

In many cases G coincides with $Aut(\Gamma)$. In such cases we write

$$Aut(\Gamma) = Aut(\Gamma_{out}) \wr Aut(\Gamma_{inn}).$$

In our example of Figure 4.6 $Aut(\Gamma_{out})$ is isomorphic to the group $H = Aut(C_4)$ which has order 8 (see below). Take triangles to realize the graphs Γ_i, $1 \leq i \leq 4$. Then $Aut(\Gamma) = H \wr S_3$, which is a group of order 20736.

In particular, we may reformulate Proposition 4.28 in terms of the wreath product in the case, when the inner graph is connected and the outer graph is a graph without edges, i. e. consists of isolated vertices only.

Proposition. *The disjoint union Γ of m isomorphic copies of a connected graph Γ_1 has automorphism group*

$$Aut(\Gamma) \simeq S_m \wr Aut(\Gamma_1).$$

For further details concerning the wreath product see for example [Hal59], [KliPR88].

4.31. Let us turn back to the question of what is $Aut(C_n)$ where as before C_n is the undirected cycle of length n. Let us consider first some particular cases. We shall assume that the vertices of C_n are numbered consecutively using $0, 1, \ldots, n-1$.

(a) $n = 3$: Here $C_3 = K_3$, the complete graph on three vertices. Clearly, every permutation of the vertex set is an automorphism. Hence, $Aut(C_3) = S_3$, and we have $|Aut(C_3)| = 6$.

The case $n = 3$ is not typical. Therefore we considere two more cases, one case in which n is even and one in which n is odd.

(b) $n = 4$: In Figure 4.7.a. there are four "rotations" $(0)(1)(2)(3), (0, 1, 2, 3), (0, 2)(1, 3)$ and $(0, 3, 2, 1)$. These four permutations are (combinatorial) automorphisms also when the graph C_4 is drawn as a polygone with different lengths of edges. Of course, in such a case they are not rotations in a geometrical sense. Nevertheless, by analogy, we continue to use the term "rotation".

Next there are two "reflections" $(0)(2)(1, 3)$ and $(0, 2)(1)(3)$. The first reflection is with respect to a line through the vertices 0 and 2. It fixes these two vertices. The second reflection is with respect to a line through the vertices 1 and 3 and fixes these vertices, too.

Further, there are "reflections" $(0, 1)(2, 3)$ and $(0, 3)(1, 2)$ with respect to the vertical and the horizontal axis, respectively (see Figure 4.7a). None of these two reflections has a fixed point. As with rotations the term "reflection" has a geometrical meaning only when the graph is represented by a regular polygon. However, we shall use this term also in the general case.

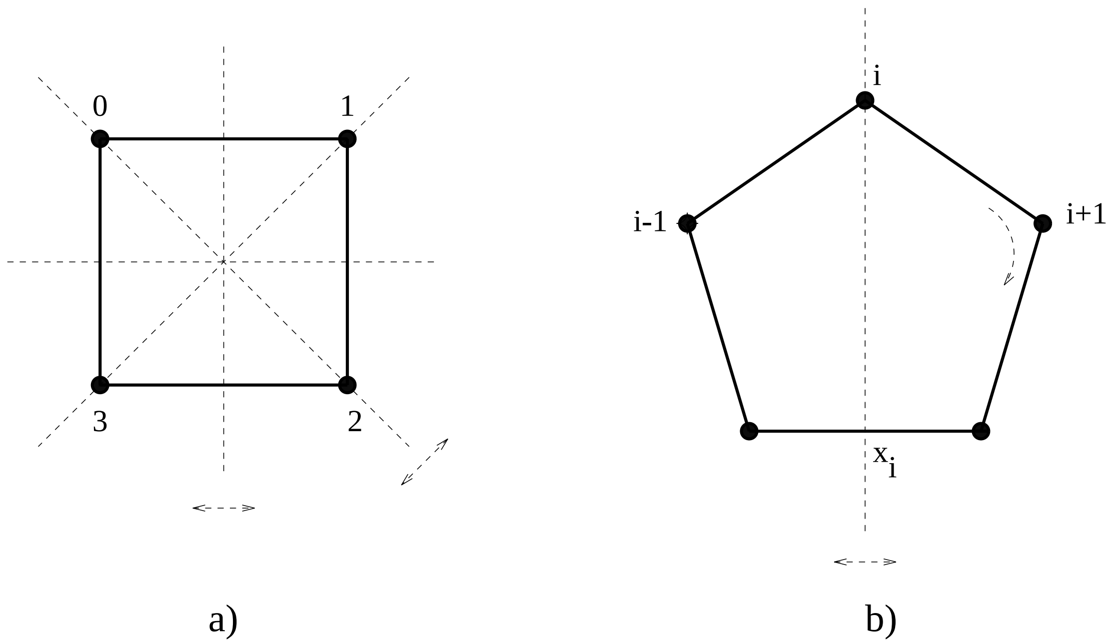


Figure 4.7.

(c) $n = 5$: This case is similar to the case $n = 4$. However, besides the rotations

$$(0)(1)(2)(3)(4), (0, 1, 2, 3, 4), (0, 2, 4, 1, 3), (0, 3, 1, 4, 2), (0, 4, 3, 2, 1)$$

there are five reflections

$$(0)(1, 4)(2, 3), (0, 2)(1)(3, 4), (0, 4)(1, 3)(2), (0, 1)(2, 4)(3), (0, 3)(1, 2)(4)$$

(see Figure 4.7b, where one of these reflections is indicated). Each reflection has exactly one fixed point. The corresponding reflection axis goes through the fixed point i and the midpoint x_i of the edge which lies "opposite" to the fixpoint.

In both cases, $n = 4$ and $n = 5$, we have n rotations and n reflections. Thus we have at least $2n$ automorphisms. In the next subsection we shall prove that there are no other automorphisms than these.

4.32. The automorphism groups of undirected cycles C_n form an important type of groups for which reason they have got a special name by which we may refer to them. There is even a special notation for them. Let

$$D_n = Aut(C_n), \ n \in \boldsymbol{N}.$$

The groups D_n are called *dihedral groups.*

Proposition. For $n \in \boldsymbol{N}$ we have $|D_n| = 2n$. Each group D_n acts transitively on the vertex set of C_n and consists of n rotations and n reflections.

Proof. Our vertex set is $\Omega_n = \{0, 1, \ldots, n-1\}$. For $i \in \Omega_n$ the mapping g_i defined for $x \in \Omega_n$ by

$$x^{g_i} = \begin{cases} x+i & \text{if } x+i < n, \\ x+i-n & \text{otherwise,} \end{cases}$$

is a rotation of C_n. Hence, we have n rotations. Further, again for $i \in \Omega_n$, the mapping h_i defined by

$$x^{h_i} = \begin{cases} 2i-x+n & \text{if } 2i-x < 0, \\ 2i-x & \text{if } 0 \leq 2i-x < n, \\ 2i-x-n & \text{otherwise,} \end{cases}$$

is a reflection. If n is odd, then all h_i are different, hence, in this case, we have n reflections. If n is even, then $h_i = h_{i+\frac{n}{2}}$. Thus, we have only $\frac{n}{2}$ reflections of this kind. Each of them has two fixed points. In addition, for n even, the mappings k_i defined by

$$x^{k_i} = \begin{cases} 2i+1-x+n & \text{if } 2i+1-x < 0, \\ 2i+1-x & \text{if } 0 \leq 2i+1-x < n, \\ 2i+1-x-n & \text{otherwise} \end{cases}$$

are reflections, too, not having any fixed point. Their number is again $\frac{n}{2}$.

So far we have seen, that D_n has at least $2n$ elements. To complete the proof we use Proposition 4.15. Since D_n acts transitively on Ω_n, we have only one orbit of cardinality n. Therefore, $|D_n| = n|(D_n)_x|$, where $x \in \Omega_n$ is arbitrary and $(D_n)_x$ is the stabilizer of x in D_n. Given x, there is only one non-trivial automorphism of C_n which fixes x, namely the reflection with respect to the axis through x. Hence $|(D_n)_x| = 2$, and we get finally $|D_n| = 2n$. ◇

For further details concerning the dihedral groups D_n consult [Hal59], [KliPR88].

5 Centralizer algebras of permutation groups

5.1. We start with a few elementary definitions. Let Ω be an arbitrary set, $g \in S(\Omega)$ and $R \subset \Omega^2$ a *binary relation on* Ω. As in Section 4, for $g \in S(\Omega)$ let $R^g = \{(x^g, y^g) : (x, y) \in \Omega^2\}$. If $R^g = R$ then R is called *invariant with respect to the permutation* g. Moreover, R is called *invariant with respect to the permutation group* (G, Ω) if $R^g = R$ for every $g \in (G, \Omega)$. If this happens, then also the graph $\Gamma = (\Omega, R)$ is said to be *invariant with respect to* (G, Ω). Let us use the notation *2-rel*(G, Ω) for the set of all binary relations on Ω which are invariant with respect to (G, Ω). Clearly, R belongs to *2-rel*(G, Ω) iff (G, Ω) is a subgroup of the automorphism group of R.

Let $\Gamma = (\Omega, R)$ and $(G, \Omega) = Aut(\Gamma)$. For every $R' \in$ *2-rel*(G, Ω) there is a corresponding graph $\Gamma' = (\Omega, R')$. Hence, *2-rel*(G, Ω) provides us with a list of all graphs having vertex set Ω which have the same (and possibly more) symmetries as Γ.

For example, consider the graph Γ in Figure 4.3 and the permutation group (H, Ω) as defined in paragraph 4.25. It was shown that Γ is invariant with respect to (H, Ω), however, H is a group of order 4, whereas the group $Aut(\Gamma)$ has order 16.

5.2. Consider again group (G, Ω) in Example 4.11. In Figure 5.1 eight graphs are given, all of which are invariant wih respect to (G, Ω), as the reader may check.

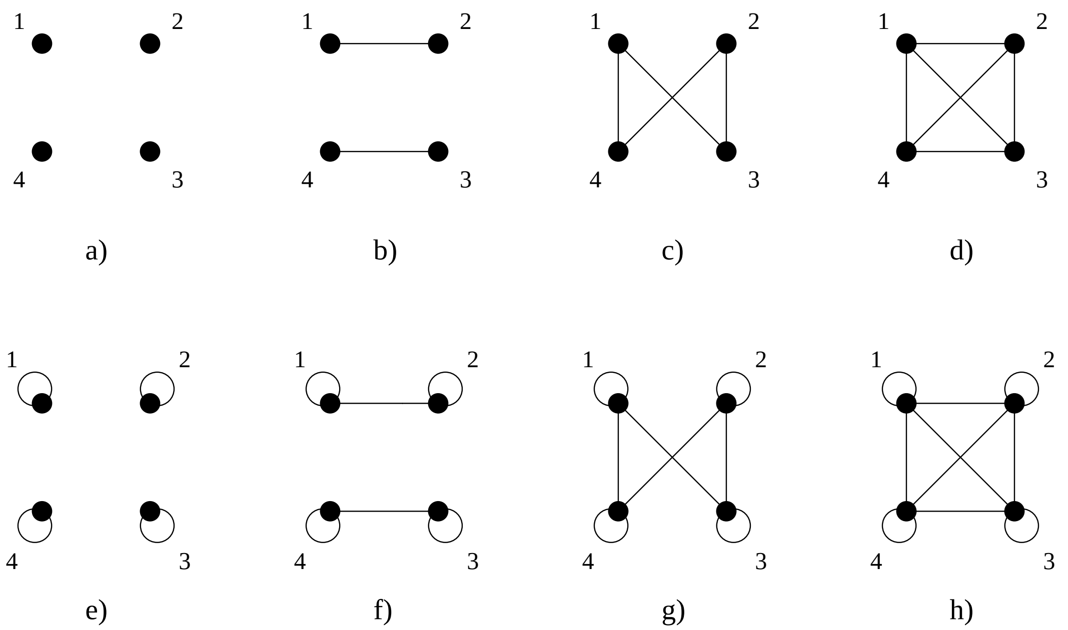


Figure 5.1.

Now, two questions arise:
(1) Is this a complete list of all graphs having this property ?
(2) Is there a simple procedure to get them all in a simple notation ?

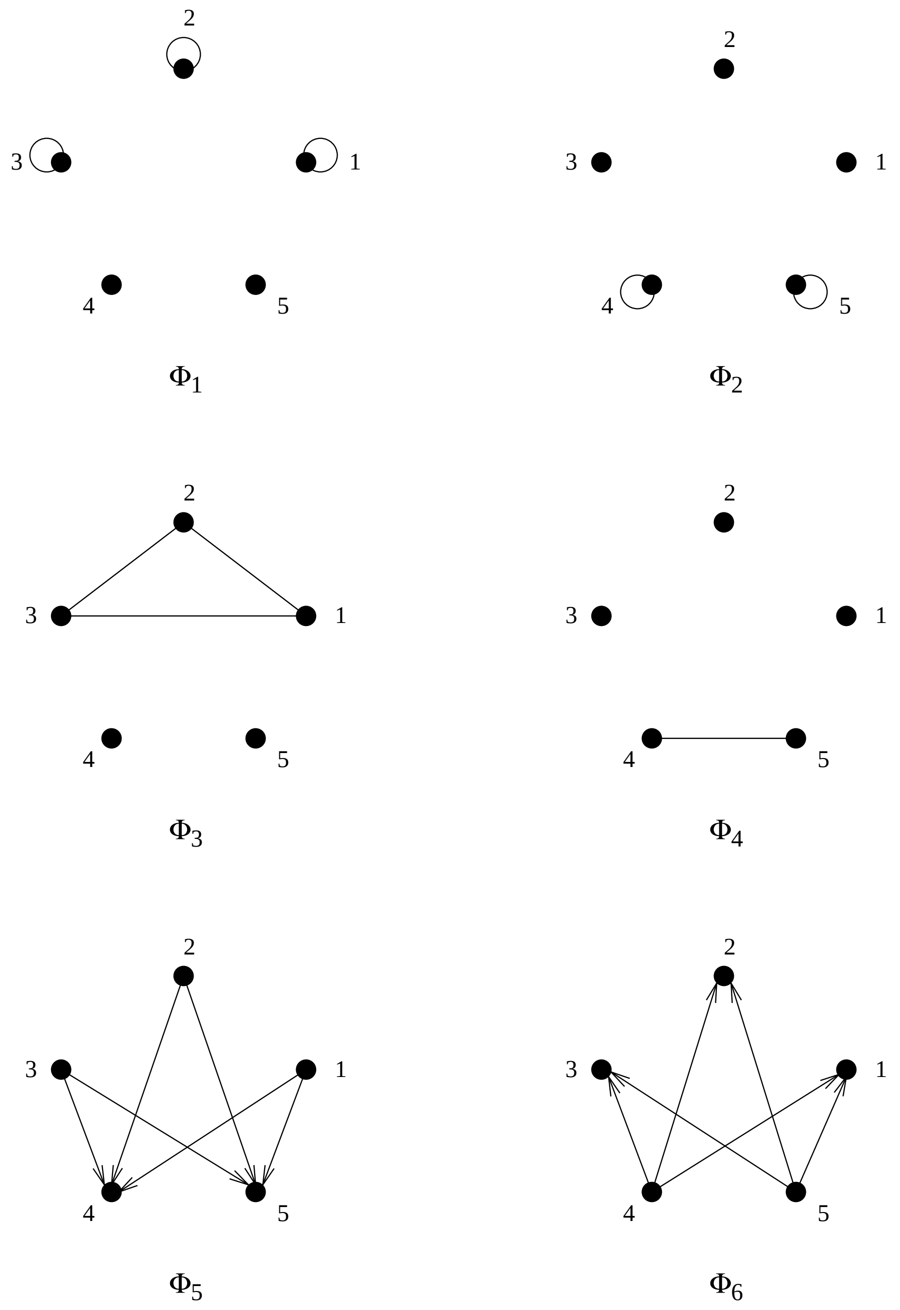


Figure 5.2.

5.3. To each permutation group (G, Ω) we can associate a new permutation group (G, Ω^2) by applying the following rule: $(a, b)^g = (a^g, b^g)$ for all $(a, b) \in \Omega^2$. [1] We say that (G, Ω^2) is *naturally induced* on the set Ω^2 by (G, Ω). The orbits of (G, Ω^2) are called *2-orbits* of (G, Ω). Thus a 2-orbit contains a pair (a, b) together with all the pairs obtainable from it by actions of permutations in G, just as an ordinary orbit (1-orbit) contains an object together with all the objects obtainable from it.

Let *2-orb*(G, Ω) be the set of all 2-orbits of (G, Ω). The set *2-orb*(G, Ω) forms a partition of Ω^2, i.e. each pair $(a, b) \in \Omega^2$ belongs to exactly one member of *2-orb*(G, Ω).

Note that each 2-orbit is a relation on Ω. A set $\Phi \in$ *2-orb*(G, Ω) is called *reflexive* if $\Phi \subset \{(a, a) : a \in \Omega\}$, otherwise Φ is called *irreflexive.* Φ is called *symmetric* if $\Phi^t = \Phi$ and Φ is called *antisymmetric* if for $a \neq b$ $(a, b) \in \Phi$ implies $(b, a) \notin \Phi$. The 2-orbits Φ and Φ^t are called *paired*, each symmetric 2-orbit is called *self-paired.*

5.4. Example:
Let us reconsider the permutation group (G, Ω) defined in paragraph 4.16. The set *2-orb*(G, Ω) is presented in Figure 5.2.

Figure 5.2 is easily constructed by
(1) writing down all possible ordered pairs of objects in Ω,
(2) writing down for each such pair those pairs which are obtained from it by the action of $g_1, \ldots, g_6$,
(3) collecting the interchangeable pairs together into sets, the 2-orbits,
(4) drawing an arc for each pair.

In our example, Φ_1 and Φ_2 are reflexive, all other 2-orbits are irreflexive. Φ_3 and Φ_4 are symmetric, Φ_5 and Φ_6 are paired antisymmetric 2-orbits.

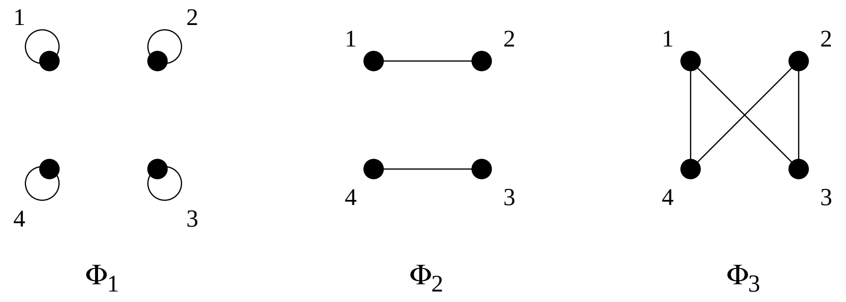


Figure 5.3.

[1] The two permutation groups (G, Ω) and (G, Ω^2) are different since they act on different sets Ω and Ω^2, respectively. Nevertheless, we denote both by the same letter G, since they are isomorphic as abstract groups, i.e. their patterns of results of the group operation ("Cayley Tables") are identical, the permutation groups are said to be different realizations of the same abstract group.

5.5. In order to be prepared for the understanding of the crucial next statement let us reconsider group (G,Ω) from 4.11. We are now able to construct the set of all 2-orbits of this group, as given in Figure 5.3. We see immediately that each invariant relation from Figure 5.1 is a union of suitable 2-orbits, e.g. the relation in Figure 5.1f is $\Phi_1 \cup \Phi_2$, the relation in Figure 5.1h is $\Phi_1 \cup \Phi_2 \cup \Phi_3$. Since there are three 2-orbits, and each 2-orbit can be selected or not selected for use in a particular union, there are eight different such unions:

$$\emptyset,\ \Phi_1,\ \Phi_2,\ \Phi_3,\ \Phi_1 \cup \Phi_2,\ \Phi_1 \cup \Phi_3,\ \Phi_2 \cup \Phi_3,\ \Phi_1 \cup \Phi_2 \cup \Phi_3.$$

(Here, $\emptyset$ means the empty relation which defines the empty graph with 4 vertices.) Generally,

$$|\mathit{2\text{-}rel}(G,\Omega)| = 2^{|\mathit{2\text{-}orb}(G,\Omega)|}.$$

5.6. As with the example in the preceding paragraph, for every permutation group (G,Ω) each invariant relation from $\mathit{2\text{-}rel}(G,\Omega)$ can be obtained as the union of suitable 2-orbits of (G,Ω). In other words, there exists a one-to-one correspondence between the elements of $\mathit{2\text{-}rel}(G,\Omega)$ and all subsets of $\mathit{2\text{-}orb}(G,\Omega)$. This fact is briefly written as follows

$$\mathit{2\text{-}rel}(G,\Omega) = 2^{\mathit{2\text{-}orb}(G,\Omega)}$$

where 2^X stands for the set of all subsets of the set X. [1]

5.7. Let (G,Ω) be defined as in the example of paragraph 5.4. Since $\mathit{2\text{-}orb}(G,\Omega)$ has 6 elements (see Figure 5.2), $\mathit{2\text{-}rel}(G,\Omega)$ has exactly 64 elements. Remember that each of these elements is a relation on Ω, and, therefore, can be considered as the arc set of a graph on Ω. Only 8 of these elements of $\mathit{2\text{-}rel}(G,\Omega)$ represent undirected graphs without loops (one of which is the empty graph).

5.8 Next we introduce a tool to represent 2-orbits conveniently. Define an $n \times n$-matrix

$$A = A(\mathit{2\text{-}orb}(G,\Omega)) = (a_{ij})$$

in the following way. For $1 \leq i,j \leq n$ let k be the number of the 2-orbit containing the pair (i,j). Define $a_{ij} = k$. In this way A becomes a matrix with integer entries storing the information which pair (i,j) belongs to which 2-orbit Φ_k. This matrix is called the *adjacency matrix* of $\mathit{2\text{-}orb}(G,\Omega)$. For example, for cuneane we obtain eighteen 2-orbits from the permutations given in 4.26 to which we assign the indices 1 through 18 in some

[1] The formal proof of this statement requires some more new notations and is therefore omitted here. However, let us demonstrate the idea of the proof reconsidering the above example. Take the invariant relation 5.1f (denoted as f for short), of which pair $(1,1)$ is an element. All pairs from the 2-orbit $Orb_G((1,1))$ belong to f. In other words, $f \supseteq \Phi_1$. Now take the difference $f^* = f \backslash \Phi_1$. $f^* \neq \emptyset$, e.g. $(1,2) \in f^*$. Therefore the 2-orbit $Orb_G((1,2))$ belongs to f^*. In other words, $f^* \supseteq \Phi_2$. Now again take the difference $f^{**} = f^* \backslash \Phi_2$, which turns out to be the empty set.

$$f^* \backslash \Phi_2 = \emptyset \Longrightarrow f^* = \Phi_2,$$
$$f^* = f \backslash \Phi_1 \Longrightarrow f = \Phi_1 \cup \Phi_2.$$

So f is a union of suitable 2-orbits.

arbitrary order. If the reflexive 2-orbits are numbered first (1 – 3), followed by the others in their natural sequence (4 – 18), then the adjacency matrix will look like

$$A = \begin{pmatrix} 1 & 4 & 5 & 6 & 6 & 5 & 4 & 7 \\ 8 & 2 & 9 & 10 & 11 & 12 & 13 & 14 \\ 14 & 9 & 2 & 10 & 11 & 13 & 12 & 8 \\ 15 & 16 & 16 & 3 & 17 & 18 & 18 & 15 \\ 15 & 18 & 18 & 17 & 3 & 16 & 16 & 15 \\ 14 & 12 & 13 & 11 & 10 & 2 & 9 & 8 \\ 8 & 13 & 12 & 11 & 10 & 9 & 2 & 14 \\ 7 & 5 & 4 & 6 & 6 & 4 & 5 & 1 \end{pmatrix}.$$

Due to the existence of antisymmetric 2-orbits in $\mathit{2\text{-}orb}(G, \Omega)$, this matrix is not symmetric. However, in chemistry we are mostly interested in symmetric 2-orbits, since e.g. the relation of atom i to atom j is considered as identical to that of atom j to atom i. Therefore, for each antisymmetric 2-orbit Φ we simply identify paired 2-orbits Φ and Φ^t. This is equivalent to looking at each twin of entries (i, j) and (j, i) in A and replacing the numerically higher entry by the lower one. The result is the adjacency matrix for the so-called symmetrified 2-orbits or briefly $\{2\}$-orbits, $\tilde{A} = A(\{\mathit{2}\}\text{-}\mathit{orb}(G, \Omega))$. In our example

$$\tilde{A} = \begin{pmatrix} 1 & 4 & 5 & 6 & 6 & 5 & 4 & 7 \\ 4 & 2 & 9 & 10 & 11 & 12 & 13 & 5 \\ 5 & 9 & 2 & 10 & 11 & 13 & 12 & 4 \\ 6 & 10 & 10 & 3 & 17 & 11 & 11 & 6 \\ 6 & 11 & 11 & 17 & 3 & 10 & 10 & 6 \\ 5 & 12 & 13 & 11 & 10 & 2 & 9 & 4 \\ 4 & 13 & 12 & 11 & 10 & 9 & 2 & 5 \\ 7 & 5 & 4 & 6 & 6 & 4 & 5 & 1 \end{pmatrix}, \quad \tilde{A}' = \begin{pmatrix} 1 & 4 & 5 & 6 & 6 & 5 & 4 & 7 \\ 4 & 2 & 9 & 10 & 11 & 12 & 13 & 5 \\ 5 & 9 & 2 & 10 & 11 & 13 & 12 & 4 \\ 6 & 10 & 10 & 3 & 8 & 11 & 11 & 6 \\ 6 & 11 & 11 & 8 & 3 & 10 & 10 & 6 \\ 5 & 12 & 13 & 11 & 10 & 2 & 9 & 4 \\ 4 & 13 & 12 & 11 & 10 & 9 & 2 & 5 \\ 7 & 5 & 4 & 6 & 6 & 4 & 5 & 1 \end{pmatrix}.$$

Matrix $\tilde{A}$ contains only thirteen different entries, $\{1, 2, 3, 4, 5, 6, 7, 9, 10, 11, 12, 13, 17\}$, and since the numbering of 2-orbits (as well as of the vertices) already is arbitrary, it is natural to renumber them in order to fill any gaps for the sake of beauty. In our example, the 17 may be replaced by 8, to obtain $\tilde{A}'$. The essential thing with these matrices ("class matrices" [RueR91b]) is that, irrespective of the particular numbers, entries representing the same $\{2\}$-orbit are identical and those representing different $\{2\}$-orbits are different. So for a molecular graph (or more exactly its automorphism group) these matrices carry the information, important to the chemist, of which atoms and which (unordered) pairs of atoms are structurally alike (are in the same class) and which are different. Some of the 2-relations also are chemically significant. Thus in the cuneane example $\Phi_4, \Phi_7, \Phi_8, \Phi_9$, and Φ_{10} (numbering of $\tilde{A}'$) taken together constitute the set of all bonds, i.e. they represent the relation "to be one another's neighbor", $\Phi_5 \cup \Phi_6 \cup \Phi_{11} \cup \Phi_{13}$ represents the relation "to be second neighbor". We will use the language of matrices in more detail later. [1]

5.9. Two permutation groups (G,Ω) and (H,Ω) are said to be *2-equivalent*, denoted by

$$(G,\Omega) \sim_2 (H,\Omega),$$

if they produce the same 2-orbits, i.e. if $\textit{2-orb}(G,\Omega) = \textit{2-orb}(H,\Omega)$. Clearly, this equality is satisfied if and only if $\textit{2-rel}(G,\Omega) = \textit{2-rel}(H,\Omega)$.

5.10. Let $\mathcal{R}$ be a set of relations on a set Ω. For each relation $R \in \mathcal{R}$ let $Aut(R)$ be its group of automorphisms. Clearly, the intersection of all these automorphism groups is again a permutation group acting on Ω (possibly the trivial group $\{e\}$). We call this intersection the *automorphism group of* $\mathcal{R}$ and denote it by

$$Aut(\mathcal{R}) = \bigcap_{R\in\mathcal{R}} Aut(R).$$

Now, let $\mathcal{R} = \textit{2-orb}(G,\Omega)$ for some arbitrary permutation group (G,Ω). In this case the group $Aut(\textit{2-orb}(G,\Omega))$ is denoted by $(G^{(2)},\Omega)$ and named "*the 2-closure* of (G,Ω)". The '2' briefly refers to the fact that it is the group of all permutations which preserve the 2-orbits of (G,Ω). We have by definition

$$(G^{(2)},\Omega) = Aut(\textit{2-orb}(G,\Omega)) = \bigcap_{\Phi\in \textit{2-orb}(G,\Omega)} Aut(\Phi).$$

5.11. Consider again the example given in 4.9. The corresponding 2-orbits, constructed in the routine manner, are shown in Figure 5.4 (top). All these 2-orbits together, each depicted in a different color, form what we call a *complete colored graph* as shown in Figure 5.4 (bottom).

The automorphism group of this complete colored graph, i.e. the group of permutations of the vertex set Ω which preserve colors on vertices as well as edges, is just the 2-closure $(G^{(2)},\Omega)$ of the initial group (G,Ω). A simple calculation shows that $|G^{(2)}| = 4$. On the other hand it is always true that $(G,\Omega) \leq (G^{(2)},\Omega)$. Taken together this means that in this case $(G^{(2)},\Omega) = (G,\Omega)$.

The proof of the following proposition is rather intricate. In a first reading it may be omitted.

[1] The number of different entries in the matrices A and $\tilde{A}$ can easily be obtained (without construction of the 2-orbits) using the Cauchy-Frobenius-Burnside Lemma. For example, the number of 2-orbits is

$$r(G,\Omega) = |\textit{2-orb}(G,\Omega)| = \frac{1}{|G|}\cdot\sum_{g\in G}\chi^2(g)$$

where $\chi(g)$ is the permutational *character* of permutation g, i.e. the number of elements in Ω which are not affected by g. In the cuneane example $r(G,\Omega) = \frac{1}{4}\cdot(8^2+2\cdot 2^2+0) = 18$. (For more details see [KliPR88], [Ker91].)

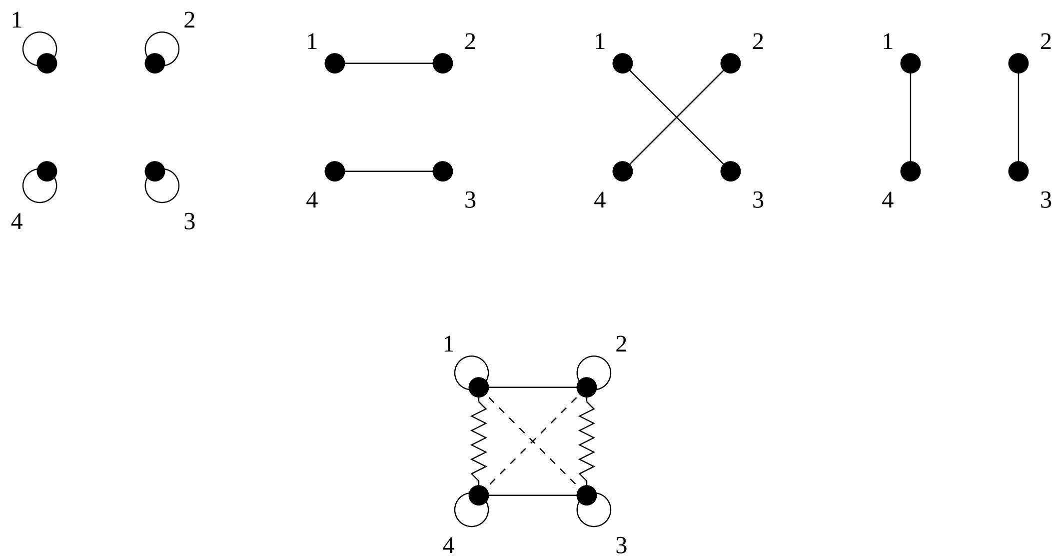


Figure 5.4.

5.12. Proposition.
(a) $(G^{(2)}, \Omega)$ *is a permutation group;*
(b) $(G^{(2)}, \Omega) \sim_2 (G, \Omega)$;
(c) if $(H, \Omega) \sim_2 (G, \Omega)$ *then* $H \leq G^{(2)}$.

Proof. (a) The intersection of any set of groups is again a group.

(b) We have $G \leq G^{(2)} \leq S(\Omega)$. This implies $\mathit{2\text{-}rel}(G^{(2)}, \Omega) \subset \mathit{2\text{-}rel}(G, \Omega)$. For arbitrary $g \in (G^{(2)}, \Omega)$ and arbitrary $\Phi \in \mathit{2\text{-}orb}(G, \Omega)$ we have $g \in Aut(\Phi)$. From this it follows that $\mathit{2\text{-}orb}(G, \Omega) \subset \mathit{2\text{-}rel}(G^{(2)}, \Omega)$, and hence, $\mathit{2\text{-}rel}(G, \Omega) \subset \mathit{2\text{-}rel}(G^{(2)}, \Omega)$. This gives finally $\mathit{2\text{-}rel}(G, \Omega) = \mathit{2\text{-}rel}(G^{(2)}\Omega)$, whence, $\mathit{2\text{-}orb}(G, \Omega) = \mathit{2\text{-}orb}(G^{(2)}, \Omega)$.

(c) Let $(H, \Omega) \sim_2 (G, \Omega)$. Then for every $R \in \mathit{2\text{-}orb}(G, \Omega)$ and for every $h \in H$ we have $R^h = R$, hence $h \in Aut(R)$. This implies $h \in (G^{(2)}, \Omega)$. Thus we have $H \leq G^{(2)}$. $\diamond$

5.13. In 5.12 we have just proved the existence of the unique largest permutation group $(G^{(2)}, \Omega)$ which is 2-equivalent to (G, Ω). A group (G, Ω) is called *2-closed* if $(G, \Omega) = (G^{(2)}, \Omega)$.

We mention the following evident properties of 2-closures:
(i) $(E^{(2)}, \Omega) = (E, \Omega)$ where $E = \{e\}$, the trivial group consisting of the identity e only;
(ii) $(S^{(2)}(\Omega), \Omega) = (S(\Omega), \Omega)$;
(iii) $(H, \Omega) \leq (G, \Omega) \Rightarrow (H^{(2)}, \Omega) \leq (G^{(2)}, \Omega)$;
(iv) $((G^{(2)})^{(2)}, \Omega) = (G^{(2)}, \Omega)$.

5.14. Let (G, Ω) be the permutation group in the example of paragraph 4.16. This group is not 2-closed, because for example the permutation $(4, 5)$ is an automorphism of every 2-orbit of (G, Ω), however $(4, 5) \notin G$. It is easy to prove that $G^{(2)} = S(\{1, 2, 3\}) + S(\{4, 5\}) =$

$S_3 + S_2$, where $S_3 + S_2$ is the group of order 12 which consists of all permutations of Ω which fix the sets $\{1, 2, 3\}$ and $\{4, 5\}$. (We have seen in 4.27 already that in the same manner, for every partition of the n-element set Ω into two parts of size k and l, $k + l = n$, the group $S_k + S_l$ can be defined. This group is the direct sum of the symmetric groups S_k and S_l, which means that all permutations within the two subsets are acting independently.)

We suggest the reader checks that in 5.11 the 2-closed permutation group (G, Ω) is not the automorphism group of any usual (non-colored) graph. So this is the smallest example showing that the term "2-closed permutation group" is more general than "automorphism group of a usual graph". Every automorphism group of a graph is 2-closed, so from a graph-theoretical point of view only 2-closed permutation groups are interesting.

5.15. Let $r = r(G, \Omega) = |\textit{2-orb}(G, \Omega)|$ be the number of distinct 2-orbits of the group (G, Ω). This number r is called the *rank* of the permutation group (G, Ω). (Sometimes the use of the term "rank" is restricted to transitive permutation groups only.) In what follows we shall reformulate the notion of invariant relations in terms of matrix language. Then, in particular, the rank of a permutation group will be interpreted as the dimension of a certain vector space associated with the group.

Recall, see 4.6, that for every permutation $g \in S(\Omega)$ there is a corresponding permutation matrix $M(g)$ of order $n = |\Omega|$. It follows from the definition of a permutation matrix that $det(M(g)) = \pm 1$. Permutations g for which $det(M(g)) = 1$ are called *even*, the others are called *odd*. The set of all even permutations on Ω forms a group $Alt(\Omega)$ of order $\frac{n!}{2}$ which is called the *alternating group* of degree n.

5.16. Let $\Gamma = (\Omega, R)$ be a graph with vertex set $\Omega = \{1, 2, \ldots, n\}$. Remember that the adjacency matrix $A(\Gamma)$ is defined as follows:

$$A(\Gamma) = (a_{ij})_{1 \leq i,j \leq n}$$

where

$$a_{ij} = \begin{cases} 1 & \text{if} \quad (i, j) \in R, \\ 0 & \text{otherwise.} \end{cases}$$

Obviously, the graph Γ is undirected iff its adjacency matrix $A(\Gamma)$ is symmetric.

The permutation matrix which corresponds to the identity permutation e on Ω is the *unit matrix* of order n, i.e. $M(e) = I_n$. Furthermore, $M(g^{-1}) = (M(g))^{-1} = (M(g))^t$, where M^t is the matrix transposed to M.

5.17. Let $D_{ij} = D_{ij}(n)$ be the matrix of order n in which the (i, j)-entry is equal to 1 and all other entries equal to 0. For example,

$$D_{23}(4) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

$D_{ij}(n)$ is the adjacency matrix of a graph with exactly one arc (i, j). Let $g \in S(\Omega)$ be such that $i^g = k, j^g = l$ and let us calculate

$$M(g^{-1})D_{ij}M(g).$$

Since there is only one non-zero entry in the column i of $M(g^{-1})$, namely in row k, we get $M(g^{-1})D_{ij} = D_{kj}$. Analogously, we find $D_{kj}M(g) = D_{kl}$. Hence $M(g^{-1})D_{ij}M(g) = D_{kl}$. Now consider $\Gamma = (\Omega, R)$. We have

$$A(\Gamma) = \sum_{(i,j)\in R} D_{ij}.$$

From this it follows

$$\begin{aligned} M(g^{-1})A(\Gamma)M(g) &= M(g^{-1})\Big(\sum_{(i,j)\in R} D_{ij}\Big)M(g) \\ &= \sum_{(i,j)\in R} M(g^{-1})D_{ij}M(g) = \\ &= \sum_{(i,j)\in R} D_{i^g j^g} = A(\Gamma^g). \end{aligned}$$

The final result is given in the following proposition.

5.18. Proposition. *Let $g \in S(\Omega)$ and $\Gamma^g = (\Omega, R^g)$. Then*

$$A(\Gamma^g) = M(g^{-1})A(\Gamma)M(g).$$

In particular $g \in Aut(\Gamma)$ if and only if

$$M(g^{-1})A(\Gamma)M(g) = A(\Gamma)$$

or

$$A(\Gamma)M(g) = M(g)A(\Gamma).$$

In other words, the permutation g is an automorphism of Γ if and only if $A(\Gamma)$ commutes with $M(g)$.

5.19. Now consider the group $M(G, \Omega) = \{M(g) : g \in G\}$ of all permutation matrices associated to the group (G, Ω). Let $\boldsymbol{Z}$ be the set of integers and $\boldsymbol{C}$ the set of complex numbers. According to what we have just observed in 5.18 a graph $\Gamma = (\Omega, R)$ is invariant with respect to (G, Ω) if and only if its adjacency matrix commutes with all permutation matrices $M(g)$, $g \in G$. This fact motivates us to consider the set $\mathcal{V}_{\boldsymbol{Z}}(G, \Omega)$ of all matrices with entries from $\boldsymbol{Z}$ which commute with all matrices $M(g)$, $g \in G$:

$$\mathcal{V}_{\boldsymbol{Z}}(G, \Omega) = \{A \in M_n(\boldsymbol{Z}) : AM(g) = M(g)A \quad \text{for all} \quad g \in (G, \Omega)\}.$$

Here $M_n(\boldsymbol{Z})$ is the set of all matrices of order n the elements of which are in $\boldsymbol{Z}$. Evidently, $\mathcal{V}_{\boldsymbol{Z}}(G, \Omega)$ is a subset of

$$\mathcal{V}_{\boldsymbol{C}}(G, \Omega) = \{A \in M_n(\boldsymbol{C}) : AM(g) = M(g)A \quad \text{for all} \quad g \in (G, \Omega)\}$$

where $M_n(\mathbb{C})$ is the set of all matrices of order n with complex-valued entries.

A set L of complex-valued matrices of order n is called a *matrix algebra* if L is closed with respect to addition and multiplication of matrices and multiplication of matrices by (complex-valued) scalars from the field $\mathbb{C}$ of complex numbers. Our set $\mathcal{V}_{\mathbb{C}}(G,\Omega)$ meets these criteria as shown below.

5.20. Proposition. *For every permutation group (G,Ω) the set $\mathcal{V}_{\mathbb{C}}(G,\Omega)$ is a matrix algebra.*

Proof. We have $A,B \in \mathcal{V}_{\mathbb{C}}(G,\Omega)$ iff $AM(g) = M(g)A$ and $BM(g) = M(g)B$ for all $g \in (G,\Omega)$. This implies

$$(A+B)M(g) = AM(g) + BM(g) = M(g)A + M(g)B = M(g)(A+B),$$
$$(AB)M(g) = A(BM(g)) = A(M(g)B) = (AM(g))B = M(g)AB,$$
$$(\lambda A)M(g) = \lambda(AM(g)) = \lambda(M(g)A) = M(g)(\lambda A)$$

for all $g \in (G,\Omega)$. Hence $A+B, AB, \lambda A \in \mathcal{V}_{\mathbb{C}}(G,\Omega)$. $\diamond$

If the same criteria are fulfilled for a set of integer matrices (multiplication restricted to scalars from $\boldsymbol{Z}$), then this set is called a *matrix ring*. In fact $\mathcal{V}_{\boldsymbol{Z}}(G,\Omega)$ is a matrix ring (as can be shown exactly as above). We call it the *centralizer ring* of (G,Ω).

5.21. The algebra $\mathcal{V}_{\mathbb{C}}(G,\Omega)$ is called the *centralizer algebra* of the permutation group (G,Ω). The notation $\mathcal{V}(G,\Omega)$ stems from the German word "Vertauschungsring" (something like "ring of commutation") which was created by I. Schur and H. Wielandt (see [Wie64]).

The centralizer algebra $\mathcal{V}_{\mathbb{C}}(G,\Omega)$ is useful when dealing with eigenvalues and eigenvectors of matrices from $\mathcal{V}_{\boldsymbol{Z}}(G,\Omega)$. If G is the automorphism group of a graph Γ then the adjacency matrix of Γ belongs to $\mathcal{V}_{\boldsymbol{Z}}(G,\Omega)$ and then the centralizer algebra yields information about the spectrum of Γ. This is an important fact, since eigenvalues of molecular graphs carry some chemical information. However, on the level of elementary combinatorial considerations, which is adopted for the present paper, the use of matrices with integer entries is sufficient. Moreover, some of these matrices have a nice graph-theoretical interpretation. [1]

[1]For some part of $\mathcal{V}_{\boldsymbol{Z}}(G,\Omega)$ a convenient interpretation can be given in terms of directed multigraphs. A *directed multigraph* $\Gamma = (\Omega, \mathcal{C})$ consists of the vertex set Ω and the function $\mathcal{C} : \Omega^2 \mapsto \boldsymbol{Z}^+ \cup \{0\}$, where the non-negative integer $\mathcal{C}(i,j)$ is the multiplicity of the arc (i,j). The multigraph Γ can be represented by its diagram or by its adjacency matrix $A(\Gamma) = (a_{ij})$ where $a_{ij} = \mathcal{C}(i,j)$.

In the same manner as for simple graphs the notion of *invariance* with respect to a given permutation group (G,Ω) can be introduced also for multigraphs. Let *2-Rel*(G,Ω) be the set of all directed multigraphs which are invariant with respect to (G,Ω). In the same manner as in 5.6 every element of *2-Rel*(G,Ω) can be interpreted as a multi-subset of *2-orb*(G,Ω). The adjacency matrices of invariant multigraphs

5.22. Proposition. *Let $\mathcal{V} = \mathcal{V}_{\mathbb{C}}(G,\Omega)$ be the centralizer algebra of the permutation group (G,Ω). Then*
(a) $\mathcal{V}$ is a vector space over the field $\mathbb{C}$;
(b) let 2-orb$(G,\Omega) = \{\Phi_1, \Phi_2, \ldots, \Phi_r\}$, $\Gamma_i = (\Omega, \Phi_i)$, $A_i = A(\Gamma_i)$ for $i \in \{1, 2, \ldots, r\}$, then the matrices $A_1, A_2, \ldots, A_r$ form a basis of the vector space $\mathcal{V}$.
(c) $dim(\mathcal{V}) = r = rank(G,\Omega)$.

Proof. Part (a) is an immediate consequence of the definition of $\mathcal{V}$ in 5.19. It follows from 5.18 and from the definition of 2-orbits that every matrix A_i, $1 \le i \le r$, belongs to $\mathcal{V}$. These matrices are evidently linearly independent. Let us show that their linear span equals $\mathcal{V}$. Let $A \in \mathcal{V}$, $A = (a_{ij})$, let $(i,j) \in \Omega^2$ and let Φ_l be the unique 2-orbit of (G,Ω) such that $(i,j) \in \Phi_l$. Moreover, let $(s,t) \in \Phi_l$. Then there exists a permutation $g \in (G,\Omega)$ such that $(i,j)^g = (s,t)$. Now use the equality $M(g)A = AM(g)$. The (i,t)-entry of $M(g)A$ is a_{ij}, whereas the (i,t)-entry of the matrix $AM(g)$ is a_{st}. We obtain $a_{ij} = a_{st}$. This means that every 2-orbit of (G,Ω) represents positions in A occupied by the same value. From this it follows that A is a linear combination of the matrices $A_1, A_2, \ldots, A_r$. Now, (c) is an evident consequence of (b). $\diamond$

5.23. The basis $A_1, A_2, \ldots, A_r$ with which the above proposition was concerned is called the *standard basis* of $\mathcal{V}_{\mathbb{C}}(G,\Omega)$. Thus for every permutation group (G,Ω) there is a standard basis of the associated centralizer algebra. To stress this fact we shall write

$$\mathcal{V}_{\mathbb{C}}(G,\Omega) = < A_1, A_2, \ldots, A_r > .$$

The 2-orbits $\Phi_1, \Phi_2, \ldots, \Phi_r$ are also called *basic relations* and the graphs $\Gamma_1, \Gamma_2, \ldots, \Gamma_r$ are called *basic graphs* of $\mathcal{V}_{\mathbb{C}}(G,\Omega)$.

Each of these three basic items carries the same information. For instance, given the basic graphs Γ_i, we may find their adjacency matrices A_i to get the standard basis, or we may write down their arc sets as relations on the vertex set to get the orbits Φ_i. The information carried by these items is which objects have symmetries realizable by action of the group G. We consider also such strange objects as matrices with complex-valued entries, because some combinatorial information is encoded even in their spectra.

5.24. Again, let (G,Ω) be a permutation group and assume $\mathcal{V}_{\mathbb{C}} = < A_1, A_2, \ldots, A_r >$, where the matrices A_i are the matrices of the standard basis. We know that $\mathcal{V}_{\mathbb{C}}(G,\Omega)$ is closed with respect to matrix multiplication. In particular, this means that the product $A_iA_j \in \mathcal{V}_{\mathbb{C}}(G,\Omega)$ for all $1 \le i,j \le r$. Every element of $\mathcal{V}_{\mathbb{C}}(G,\Omega)$ is uniquely expressable as a linear combination of the basic matrices. Hence,

$$A_iA_j = \sum_{k=1}^{r} p_{ij}^k A_k$$

are just the matrices in $\mathcal{V}_{\boldsymbol{Z}}(G,\Omega)$ which have non-negative entries. Hence, the proof of Proposition 5.21 can be considered as a more refined and more rigorous version of the reasoning in 5.6. We shall see from our further considerations that matrix and relational languages are exchangeable in the treatment of centralizer rings. A suitable combination of these two languages will help us to realize more vividly the basic ideas of centralizer ring theory.

for all $1 \le i, j \le r$. The 3-dimensional tensor $(p_{ij}^k)_{1 \le i,j,k \le r}$ is called the *tensor of structure constants* of the centralizer algebra $\mathcal{V}_{\mathbb{C}}(G, \Omega)$. (Here k is not an exponent but an index, written as a superscript for better legibility.)

Note that all structure constants are non-negative integers. Indeed, since every basic matrix is a $(0,1)$-matrix, each of the products $A_i A_j$ has non-negative integral entries only. For every (s,t)-entry of $A_i A_j$ there is exactly one basic matrix, say A_k, the (s,t)-entry of which is non-zero (and therefore equals 1). This implies that

$$p_{ij}^k = (A_i A_j)_{st}.$$

Hence, p_{ij}^k is a non-negative integer.

5.25. Let us switch back from matrix language to the language of relations in order to obtain a combinatorial interpretation of the structure constants.

First, let us introduce a compact description of centralizer algebras. Let $\Gamma_1, \Gamma_2, \ldots, \Gamma_r$ be the basic graphs of $\mathcal{V}_{\mathbb{C}}(G, \Omega)$. The arc sets of these graphs form a partition of Ω^2. Let us color the arcs of Γ_i with color i, $1 \le i \le r$. Then, instead of $\Gamma_1, \Gamma_2, \ldots, \Gamma_r$ we can speak of the *complete colored graph* $\Gamma = \Gamma(\mathcal{V}_{\mathbb{C}}(G, \Omega))$. Each arc of this complete graph is colored by exactly one of the colors in $\{1, 2, \ldots, r\}$. In addition, we associate to Γ its *generalized adjacency matrix*

$$A = A(\mathcal{V}_{\mathbb{C}}(G, \Omega)) = \sum_{k=1}^{r} k A_k,$$

where each (s,t)-entry of A is equal to the color of the arc (s,t) in Γ. The matrix A is perhaps the most compact way for the description of $\mathcal{V}_{\mathbb{C}}(G, \Omega)$. Note that A is independent of what we use as the underlying set of scalars, $\mathbb{C}$ or $\mathbb{Z}$. Hence, $A(\mathcal{V}_{\mathbb{C}}(G, \Omega)) = A(\mathcal{V}_{\mathbb{Z}}(G, \Omega))$. For this reason, we often suppress the subscripts and denote this matrix more simply by $A(\mathcal{V}(G, \Omega))$.

5.26. Let (s,t) be an arc of color k in Γ. This means in other words,

$$(A_k)_{st} = 1, \ (A_i)_{st} = 0 \quad \text{for} \quad i \ne k.$$

Let us select two colors i and j and let us consider the number γ_{ij}^k of walks (s,x,t) of length 2 from s to t which use an arc (s,x) of color i followed by an arc (x,t) of color j. It follows immediately from the rules for matrix multiplication that γ_{ij}^k is equal to the (s,t)-entry in $A_i A_j$. As shown in 5.24, this entry is p_{ij}^k. Hence, $\gamma_{ij}^k = p_{ij}^k$, and we see that the structure constant p_{ij}^k is equal to the number of triangles (s,x,t) which occur in the colored graph Γ having a fixed "basic" arc (s,t) of color k and having arcs (s,x) and (x,t) of color i and color j, respectively. This number is independent of how we select the arc (s,t) of color k, therefore, it is an invariant of the set of arcs of color k in Γ.

The combinatorial interpretation of the structure constants given here is sometimes very helpful for the computation of the tensor (p_{ij}^k) which belongs to a given centralizer algebra

$\mathcal{V}_{\mathfrak{C}}(G, \Omega)$.

5.27. If (G, Ω) is a transitive permutation group then, by convention, the relations in *2-orb*(G, Ω) are numbered using the index set $\{0, 1, \ldots, r-1\}$. Also by convention, $\Phi_0 = \{(i,i) | i \in \Omega\}$, the *diagonal* of Ω^2 which is the only *reflexive 2-orbit* in *2-orb*(G, Ω). The arc set of the corresponding basic graph consists of loops attached to all the vertices in Ω. According to this convention the entries of the adjacency matrix A of the colored graph Γ range from 0 to $r-1$.

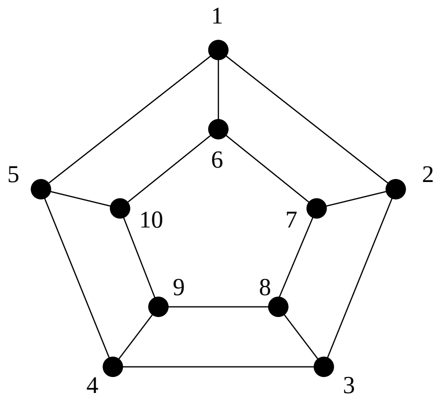


Figure 5.5.

5.28. Example:
Let us consider the regular *pentagonal prism* (see Figure 5.5). The corresponding hydrocarbon was synthesized [EatOB81]. It is well-known that its complete symmetry group is D_{5h} (see, e.g. [Ham62]) and has order 20. This point group has an isomorphic representation as a transitive permutation group of order 20 acting on a set of cardinality 10. It is the automorphism group of the graph associated with the pentagonal prism P_{10}. Let

$\Omega = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$,
$G = < g_1, g_2, g_3 >$ where
$g_1 = (1, 2, 3, 4, 5)(6, 7, 8, 9, 10)$, $g_2 = (2, 5)(3, 4)(7, 10)(8, 9)$,
$g_3 = (1, 6)(2, 7)(3, 8)(4, 9)(5, 10)$.

The reader will be able to check that

$$\textit{2-orb}(G, \Omega) = \{\Phi_0, \Phi_1, \Phi_2, \Phi_3, \Phi_4, \Phi_5\}$$

where all relations Φ_i, $0 \leq i \leq 5$, are depicted in Figure 5.6.

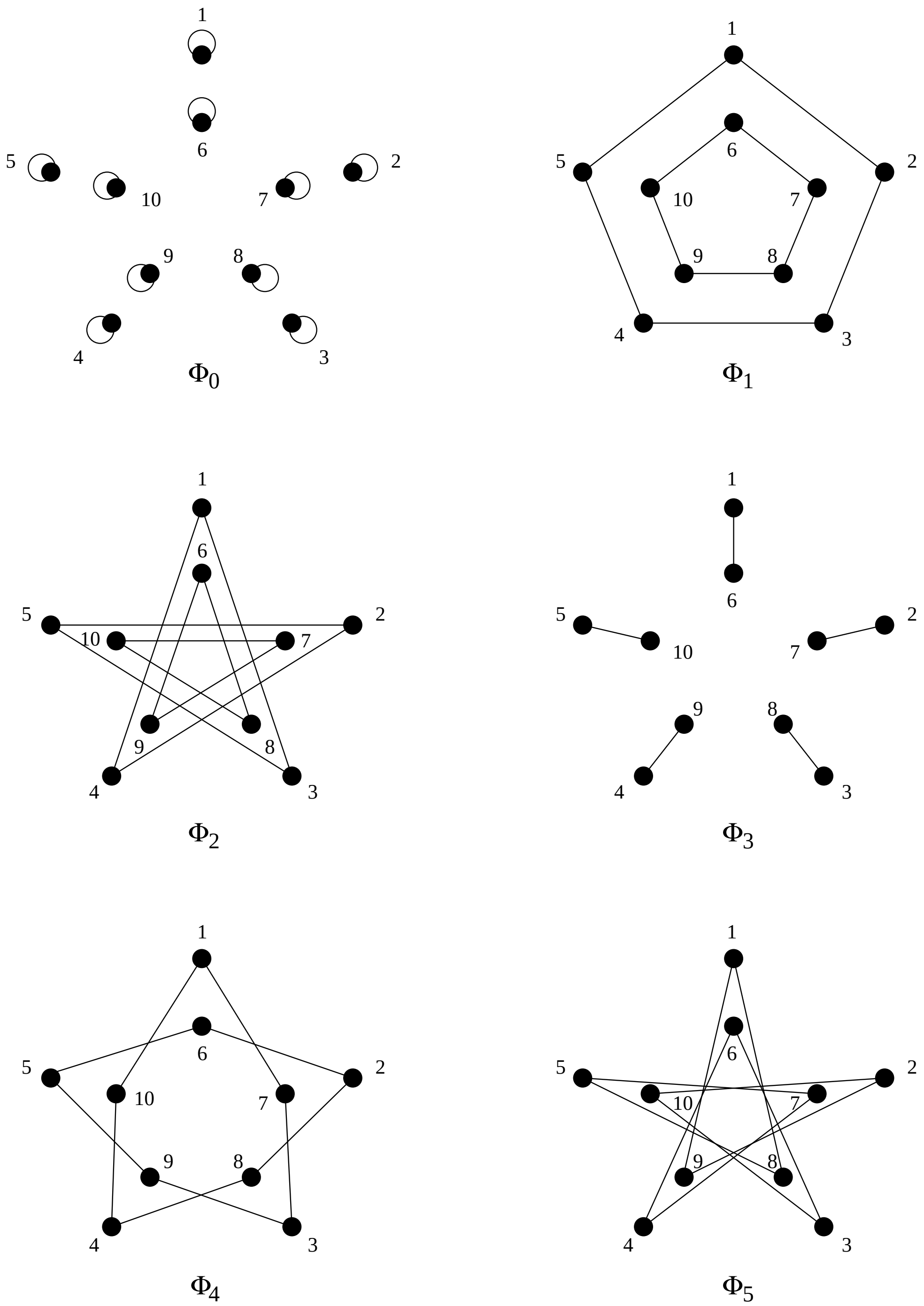

1 6 5 2 10 7 9 8 4 3
Φ_0
1 5 6 2 10 7 9 8 4 3
Φ_1
1 6 5 2 10 7 9 8 4 3
Φ_2
1 6 5 2 10 7 9 8 4 3
Φ_3
1 5 6 2 10 7 9 8 4 3
Φ_4
1 6 5 2 10 7 9 8 4 3
Φ_5

Figure 5.6.

The graph P_{10} is invariant with respect to (G, Ω), hence its arc set is a union of 2-orbits, $\Phi_1 \cup \Phi_3$. The adjacency matrix $A = A(\mathcal{V}(G, \Omega))$ can be immediately obtained from the 2-orbits in Figure 5.5:

$$A = \begin{pmatrix} 0 & 1 & 2 & 2 & 1 & 3 & 4 & 5 & 5 & 4 \\ 1 & 0 & 1 & 2 & 2 & 4 & 3 & 4 & 5 & 5 \\ 2 & 1 & 0 & 1 & 2 & 5 & 4 & 3 & 4 & 5 \\ 2 & 2 & 1 & 0 & 1 & 5 & 5 & 4 & 3 & 4 \\ 1 & 2 & 2 & 1 & 0 & 4 & 5 & 5 & 4 & 3 \\ 3 & 4 & 5 & 5 & 4 & 0 & 1 & 2 & 2 & 1 \\ 4 & 3 & 4 & 5 & 5 & 1 & 0 & 1 & 2 & 2 \\ 5 & 4 & 3 & 4 & 5 & 2 & 1 & 0 & 1 & 2 \\ 5 & 5 & 4 & 3 & 4 & 2 & 2 & 1 & 0 & 1 \\ 4 & 5 & 5 & 4 & 3 & 1 & 2 & 2 & 1 & 0 \end{pmatrix}.$$

The structure constants p_{ij}^k are obtained by a simple two-step operation. First each product of two basic matrices is written as a linear combination of basic matrices, using Figure 5.6. Thus applying A_1 two times is equivalent to walking from vertex 1 to vertex 2 and thence to vertex 3 or back to 1 (Φ_1), or from 1 to 5 and thence to 4 or back to 1. So 1 is arrived at from 1 twice (Φ_0), 3 and 4 are reached once (Φ_2). This is written as

$$A_1^2 = 2A_0 + A_2.$$

Similarly,

$$\begin{aligned} A_1 A_2 &= A_2 A_1 = A_1 + A_2, \\ A_1 A_3 &= A_3 A_1 = A_4, \\ A_1 A_4 &= A_4 A_1 = 2A_3 + A_5, \\ A_1 A_5 &= A_5 A_1 = A_4 + A_5, \\ A_1 A_0 &= A_0 A_1 = A_1, \quad \text{etc.} \end{aligned}$$

Second, by definition the p_{ij}^k's are the coefficients in this system of equations, i.e.

$$p_{11}^0 = 2,\ p_{11}^1 = 0,\ p_{11}^2 = 1,\ p_{11}^3 = p_{11}^4 = p_{11}^5 = 0,$$

$$p_{12}^0 = 0,\ p_{12}^1 = p_{12}^2 = 1,\ p_{12}^3 = p_{12}^4 = p_{12}^5 = 0,$$
$$p_{21}^k = p_{12}^k \quad \text{for} \quad 0 \le k \le 5, \quad \text{etc.}$$

In the same manner all other constants can be calculated. (We shall return to this example in Section 9). [1]

[1] The notions of centralizer algebra and centralizer ring of a transitive permutation group can be introduced using double cosets of the group G with respect to its stabilizer G_x of an arbitrary element $x \in \Omega$. In this representation the centralizer algebra is well-known in algebraic combinatorics as the *Hecke algebra*. For more details see [FarKM94].

6 Cellular algebras

6.1. Let $\mathcal{W} \subset M_n(\mathbb{C})$ be a matrix algebra over $\mathbb{C}$ such that the following requirements are fulfilled:

(CA1) Considered as a linear space over $\mathbb{C}$ the algebra $\mathcal{W}$ has some basis $A_1, A_2, \ldots, A_r$, where $A_i,\ 1 \leq i \leq r$, is a set of $(0,1)$-matrices;

(CA2) $\sum_{i=1}^{r} A_i = J_n$, where J_n is the matrix of order n all entries of which are equal to 1;

(CA3) For every $i \in \{1, 2, \ldots, r\}$ there is an $i' \in \{1, 2, \ldots, r\}$ such that $A_i^t = A_{i'}$.

Then $\mathcal{W}$ is called a *cellular algebra of rank* r *and order* n with *standard basis* $A_1, A_2, \ldots, A_r$, and we shall indicate this fact by writing

$$\mathcal{W} = < A_1, A_2, \ldots, A_r > .$$

Most frequently only the case of cellular algebras with *unit element* is considered, i.e. algebras that fulfill the additional requirement:

(CA4) The unit matrix I_n belongs to $\mathcal{W}$.

However, we stress that cellular algebras which do not satisfy (CA4) are also important for describing and analyzing combinatorial structures.

A ring of matrices which is closed with respect to multiplying matrices by scalars from $\boldsymbol{Z}$ is called a $\boldsymbol{Z}$-module. If $\mathcal{W}$ is a cellular algebra then its intersection with $M_n(\boldsymbol{Z})$ (the set of all matrices of order n with entries from $\boldsymbol{Z}$) is a $\boldsymbol{Z}$-module. Since this ring contains the standard basis $A_1, A_2, \ldots, A_r$, it also fulfils the axioms (CA1) - (CA4), provided that in (CA1) the field $\mathbb{C}$ is replaced by the ring $\boldsymbol{Z}$. A matrix ring with this property is called a *cellular ring* with or without unit element, depending on the validity of (CA4). We shall use the same notation

$$\mathcal{W} = < A_1, A_2, \ldots, A_r >$$

for the cellular algebra and for the cellular ring with the same standard basis. As mentioned in the previous section, if we restrict ourselves to a combinatorial point of view (and spectral properties of matrices from $\mathcal{W}$ are not required) then it is sufficient to consider cellular rings only.

Double cosets (without reference to Hecke algebras) and their use in group-theoretical models are also known in mathematical chemistry, see e.g. [BroHM74], [RucK83], [BroGW83], [DugKMU84], [Has85]. An excellent presentation of the double coset approach within the framework of algebraic combinatorics can be found in [Ker91].

We intend to discuss the interrelations between 2-orbits of permutation groups and double cosets in one of the subsequent papers in this series.

In a purely combinatorial approach like here the use of double cosets does not give any essential advantages. For this reason we avoid their use in the current presentation.

A cellular algebra $\mathcal{W}$ is called a *cell* if there exist numbers $n_1, \ldots, n_r$ such that in each basic matrix A_i, $1 \leq i \leq r$, the number of ones in each row is n_i. In the case of cells with unit, by convention, we set $A_0 = I_n$ and use the index set $\{0, 1, \ldots, r-1\}$ for numbering the basic matrices.

6.2. Let (G, Ω) be an arbitrary permutation group. The centralizer algebra (ring) of (G, Ω) is an example for a cellular algebra (ring), respectively. Certainly, (CA1) - (CA4) are satisfied for any centralizer algebra (ring). However, it is not true that every cellular algebra coincides with the algebra $\mathcal{V}_{\mathbb{C}}(G, \Omega)$ for a suitable group (G, Ω). A few examples will be considered in the course of our presentation.

6.3. The term "cellular algebra" goes back to the Soviet School of algebraic combinatorics. It was introduced by B. Ju. Weisfeiler and A. A. Leman in [WeiL68], see also [Wei76]. One of the pioneers in the application of centralizer rings of permutation groups was D.G. Higman, see his classical paper [Hig64]. Higman called matrix algebras which satisfy (CA1) - (CA4) *coherent algebras* (see [Hig87] or [BanI84] for a more modern presentation). Nowadays, in western literature the term coherent algebra is widely adopted. The particular case of coherent algebras which are equivalent to cells with unit is well-known in the literature as *BM–algebras (Bose–Mesner algebras)* of *association schemes* (see e.g. [BanI84]).

The main lines of the historical development of all these and other notions will be discussed in Section 10.

6.4. In this paragraph we consider a non-standard matrix multiplication which is called *Schur-Hadamard multiplication*. Let $A = (a_{ij})$ and $B = (b_{ij})$ be two square matrices of order n and define

$$c_{ij} = a_{ij} b_{ij},\ 1 \leq i, j \leq n.$$

The matrix $C = (c_{ij})$ is called the *Schur-Hadamard product* of A and B and is denoted by $C = A \circ B$.

It turns out that every cellular algebra (ring) is closed with respect to this componentwise multiplication of matrices. To see this let us look at the Schur-Hadamard products (S-H product for short) of basic matrices. Let $\mathcal{W} = < A_1, A_2, \ldots, A_r >$. It follows immediately from (CA1) and (CA2) that $A_i \circ A_i = A_i$ for all $1 \leq i \leq r$ and $A_i \circ A_j = O$ for all $1 \leq i \neq j \leq r$, where O denotes the matrix of order n all of whose entries are equal to 0. Now, taking into account that every element of $\mathcal{W}$ is representable as a linear combination of the matrices $A_1, A_2, \ldots, A_r$, we immediately see that $\mathcal{W}$ is indeed closed with respect to $\circ$.

The closedness of $\mathcal{W}$ with respect to S-H-multiplication is, in our opinion, the most essential additional property by which cellular algebras are distinguished from ordinary matrix algebras. All advantages of using the two kinds of multiplications within one algebraic structure become apparent in the so-called duality theory for commutative cells (see [BanI84]). Within the frame of our elementary exposition we shall demonstrate only a certain simple combinatorial application of the S-H-multiplication which is nevertheless rather impressive.

6.5. Schur - Wielandt principle. *Let $\mathcal{W} = <A_1, A_2, \ldots, A_r>$ be a cellular algebra of order n and let $X = (x_{ij}) \in \mathcal{W}$. For arbitrary $\nu \in \mathbb{C}$ define $Y = Y(\nu, X)$ (cross–section of X by ν) by*

$$y_{ij} = \begin{cases} \nu & \text{if} \quad x_{ij} = \nu, \\ 0 & \text{otherwise.} \end{cases}$$

We have $Y(\nu, X) \in \mathcal{W}$ for all $\nu \in \mathbb{C}$.

Proof. If $\nu = 0$ or if ν is not equal to some entry of X then $Y(\nu, X) = O \in \mathcal{W}$. Therefore, let us consider the case where $\nu \neq 0$ equals some entry of X. Assume $\nu = x_{st}$. Let k_1 be such that the basic matrix A_{k_1} satisfies $(A_{k_1})_{st} = 1$. Define $Z_1 = X \circ A_{k_1}$. We have $Z_1 \in \mathcal{W}$. Since Z_1 has non-zero entries only on those places where A_{k_1} has 1's, we must have $Z_1 = \nu A_{k_1}$.

Now, continue with the matrix $T_1 = X - Z_1$ which also belongs to $\mathcal{W}$. T_1 has the same entries as X on all positions except those which are occupied by 1's in A_{k_1}. If at least one entry in T_1 equals ν then we apply the same procedure to T_1 instead of X thereby obtaining matrices $Z_2 = \nu A_{k_2}$ and $T_2 = T_1 - Z_2$. This process will terminate after some finite number $q \geq 1$ of steps, and we obtain finally

$$\begin{aligned} Y(\nu, X) &= Z_1 + Z_2 + \ldots + Z_q = \\ &= \nu(A_{k1} + A_{k_2} + \ldots + A_{k_q}). \end{aligned}$$

◇

6.6. Corollary. *Under the same assumptions as in 6.5 the following assertion holds for all $\nu \in \mathbb{C}$, $\nu \neq 0$: For every matrix $X \in \mathcal{W}$ there exists a subset $K = \{k_1, k_2, \ldots, k_q\}$ of $\{1, 2, \ldots, r\}$ such that*

$$\frac{1}{\nu} Y(\nu, X) = \sum_{k_i \in K} A_{k_i}.$$

6.7. Let Ω be a set and $\mathcal{R} = \{R_1, R_2, \ldots, R_r\}$ and $\mathcal{S} = \{S_1, S_2, \ldots, S_s\}$ be two partitions of Ω. $\mathcal{R}$ is called *finer* than $\mathcal{S}$ if every class of $\mathcal{S}$ is a union of some classes of $\mathcal{R}$. In this case $\mathcal{S}$ is also called *coarser* than $\mathcal{R}$.

The *join* $\mathcal{T} = \mathcal{R} \vee \mathcal{S}$ *of two partitions* $\mathcal{R}$ and $\mathcal{S}$ of a set Ω is defined as the finest partition of Ω which is coarser than $\mathcal{R}$ and coarser than $\mathcal{S}$. It is obvious from the definition of $\mathcal{T}$ that if $R_i \cap S_j$ is non-empty then $R_i \cup S_j$ must be completely contained in some class T_k of $\mathcal{T}$. Hence, for finding the classes of $\mathcal{T}$ we may use the following auxiliary graph $\Pi = (V, E)$ where $V = \{x_1, \ldots, x_r\} \cup \{y_1, \ldots, y_s\}$ and where E is a set of undirected edges $\{x_i, y_j\}$ defined by $\{x_i, y_j\} \in E$ if and only if $R_i \cap S_j \neq \emptyset$. The vertices x_i in Π correspond to the classes R_i, the vertices y_j correspond to the classes S_j. Now, let $\Pi_1, \ldots, \Pi_t$ be the connected components of Π. Then $\mathcal{T}$ has classes T_k, $1 \leq k \leq t$, where

$$T_k = \bigcup_{x_i \in \Pi_k} R_i = \bigcup_{y_j \in \Pi_k} S_j.$$

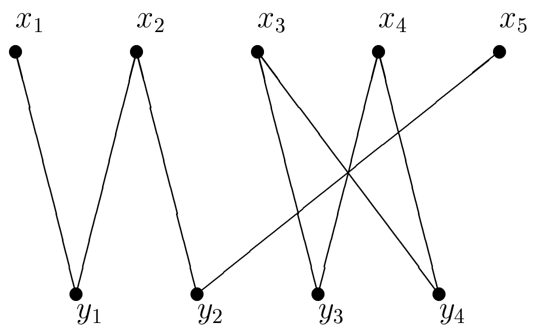


Figure 6.1.

To have an example, consider the two partitions

$$\mathcal{R} = \{a\},\ \{b,c\},\ \{d,e\},\ \{f,g\},\ \{h\}$$

and

$$\mathcal{S} = \{a,b\},\ \{c,h\},\ \{d,f\},\ \{e,g\}$$

of $\{a,b,c,d,e,f,g,h\}$. The corresponding graph Π is depicted in Figure 6.1. Π contains two connected components. Hence, $\mathcal{R} \vee \mathcal{S}$ consists of two classes T_1 and T_2 where

$$T_1 = \{a,b,c,h\} \quad \text{and} \quad T_2 = \{d,e,f,g\}.$$

6.8. For $A \in M_n(\mathbb{C})$ define the relation $supp(A)$ on the set $\Omega = \{1,2,\ldots,n\}$ by

$$(i,j) \in supp(A) \Leftrightarrow a_{ij} \neq 0.$$

The relation $supp(A)$ is usually called the *support* of the matrix A. For the cellular algebra $\mathcal{W} = \langle A_1, A_2, \ldots, A_r \rangle$ let $R_i = supp(A_i)$, $1 \leq i \leq r$. The relations R_i are called *basic relations* for W, the graphs $(\{1,2,\ldots,n\}, R_i)$ are called *basic graphs.* Due to (CA2), the basic relations define a partition of Ω^2.

Let $\mathcal{W}_1 = \langle A_1, A_2, \ldots, A_r \rangle$ and $\mathcal{W}_2 = \langle B_1, B_2, \ldots, B_s \rangle$ be two cellular algebras of the same order n. Then we may consider their usual set-theoretical *intersection* $\mathcal{W}_1 \cap \mathcal{W}_2$. To find out what $\mathcal{W}_1 \cap \mathcal{W}_2$ is like consider the following procedure:
(i) construct the basic relations $R_1, R_2, \ldots, R_r$ and $S_1, S_2, \ldots, S_s$ for $\mathcal{W}_1$ and $\mathcal{W}_2$, respectively;
(ii) construct the join $\mathcal{T} = \{T_1, T_2, \ldots, T_t\}$ of the partitions $\mathcal{R} = \{R_1, R_2, \ldots, R_r\}$ and $\mathcal{S} = \{S_1, S_2, \ldots, S_s\}$ of Ω^2.
(iii) find the adjacency matrices $C_i = A(\Gamma_i)$, $\Gamma_i = (\Omega, T_i)$, $1 \leq i \leq t$;
(iv) construct the linear subspace $\langle C_1, C_2, \ldots, C_t \rangle$ of $M_n(\mathbb{C})$.

6.9. Proposition. *Let $\mathcal{W}_1 = \langle A_1, A_2, \ldots, A_r \rangle$ and $\mathcal{W}_2 = \langle B_1, B_2, \ldots, B_s \rangle$ be cellular algebras of the same order n. Then $\mathcal{W}_1 \cap \mathcal{W}_2$ is also a cellular algebra, and we have*

$$\mathcal{W}_1 \cap \mathcal{W}_2 = \langle C_1, C_2, \ldots, C_t \rangle .$$

Proof. The first part of the statement is rather evident. Indeed, the proof is absolutely trivial if the following fact is considered: a subspace $\mathcal{W}$ of $M_n(\mathbb{C})$ is a cellular algebra if

$\mathcal{W}$ is closed with respect to usual matrix multiplication as well as to Schur-Hadamard multiplication, if it is closed with respect to taking the conjugate transposed of its matrices, and finally if it contains the matrices J_n and I_n (in the case of (CA4)). Since each of the algebras $\mathcal{W}_1$ and $\mathcal{W}_2$ has these properties, clearly, $\mathcal{W}_1 \cap \mathcal{W}_2$ possesses them, too.

To complete the proof we have to check that $\mathcal{W}_1 \cap \mathcal{W}_2$ equals the linear span of the matrices $C_1, C_2, \ldots, C_t$. This follows from the definition of the join of the two partitions $\mathcal{R}$ and $\mathcal{S}$. By definition, for each k, $1 \leq k \leq t$, there are subsets $U_k \subseteq \{1, 2, \ldots, r\}$ and $V_k \subseteq \{1, 2, \ldots, s\}$ with

$$T_k = \bigcup_{i \in U_k} R_i = \bigcup_{j \in V_k} S_j.$$

Hence

$$C_k = \sum_{i \in U_k} A_i = \sum_{j \in V_k} B_j.$$

This implies $C_k \in \mathcal{W}_1 \cap \mathcal{W}_2,\ 1 \leq k \leq t$. Hence $< C_1, \ldots, C_t > \subseteq \mathcal{W}_1 \cap \mathcal{W}_2$.

On the other hand, if $A \in \mathcal{W}_1 \cap \mathcal{W}_2$, then there exist coefficients $\lambda_i, \mu_j \in \mathbb{C}$ such that

$$A = \sum_{i=1}^{r} \lambda_i A_i = \sum_{j=1}^{s} \mu_j B_j.$$

Because of $A = A \circ J$ and $J = \sum_{i=1}^{r} A_i = \sum_{j=1}^{s} B_j$ we find

$$A = \sum_{i=1}^{r} \sum_{j=1}^{s} \lambda_i (A_i \circ B_j) = \sum_{j=1}^{s} \sum_{i=1}^{r} \mu_j (A_i \circ B_j).$$

Obviously, $A_i \circ B_j \neq O$ implies $\lambda_i = \mu_j$. Let us use once more the auxiliary graph $\Pi = (V, E)$ defined in subsection 6.7 for the partitions $\mathcal{R}$ and $\mathcal{S}$. Note that $R_i \cap S_j \neq \emptyset$ if and only if $A_i \circ B_j \neq 0$. Therefore, it is clear that $\lambda_i = \mu_j$ whenever x_i and y_j belong to the same component Π_k of Π. Hence, $\lambda_i = \mu_j$ for all $(i, j) \in U_k \times V_k$. Write ν_k for this common value of λ_i and μ_j, which depends on k only. Then

$$A = \sum_{k=1}^{t} \sum_{(i,j) \in U_k \times V_k} \lambda_i (A_i \circ B_j) = \sum_{k=1}^{t} \nu_k C_k.$$

This proves $\mathcal{W}_1 \cap \mathcal{W}_2 \subseteq < C_1, \ldots, C_t >$. ◇

6.10. EXAMPLE:
Consider the graph Γ in Figure 6.2, which consists of the vertices and edges of an octahedron. The permutations $g = (2, 3, 4, 5)$ and $h = (1, 2, 3)(4, 5, 6)$ are automorphisms of Γ. Let us consider the cyclic groups $G =< g >= \{g, g^2, g^3, g^4 = e\}$ and $H =< h >= \{h, h^2, h^3 = e\}$ acting as permutation groups on the same set $\Omega = \{1, 2, 3, 4, 5, 6\}$. Let $\mathcal{W}_1 = \mathcal{V}_{\mathbb{C}}(G, \Omega), \mathcal{W}_2 = \mathcal{V}_{\mathbb{C}}(H, \Omega)$. These two cellular algebras (which are also centralizer

algebras) are represented by the following two adjacency matrices of the corresponding colored graphs:

$$A_1 = \begin{pmatrix} 1 & 4 & 4 & 4 & 4 & 5 \\ 6 & 2 & 7 & 8 & 9 & 10 \\ 6 & 9 & 2 & 7 & 8 & 10 \\ 6 & 8 & 9 & 2 & 7 & 10 \\ 6 & 7 & 8 & 9 & 2 & 10 \\ 11 & 12 & 12 & 12 & 12 & 3 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 3 & 1 & 2 & 6 & 4 & 5 \\ 2 & 3 & 1 & 5 & 6 & 4 \\ 7 & 8 & 9 & 12 & 10 & 11 \\ 9 & 7 & 8 & 11 & 12 & 10 \\ 8 & 9 & 7 & 10 & 11 & 12 \end{pmatrix}.$$

Here we use the agreements about notation which were established in 5.8, by coincidence both algebras have rank equal to 12. Using the procedure described in 6.8 we obtain the adjacency matrix A of the intersection $\mathcal{W}_1 \cap \mathcal{W}_2$:

$$A = \begin{pmatrix} 1 & 2 & 2 & 2 & 2 & 3 \\ 2 & 1 & 2 & 3 & 2 & 2 \\ 2 & 2 & 1 & 2 & 3 & 2 \\ 2 & 3 & 2 & 1 & 2 & 2 \\ 2 & 2 & 3 & 2 & 1 & 2 \\ 3 & 2 & 2 & 2 & 2 & 1 \end{pmatrix}.$$

It is well known that $|Aut(\Gamma)| = 48$ (see also Example 7.4), and it is easy to see that $\mathcal{W}_1 \cap \mathcal{W}_2 = \mathcal{V}_{\mathbb{C}}(Aut(\Gamma), \Omega)$.

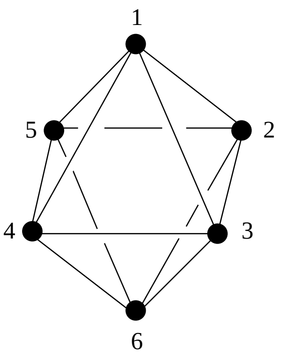


Figure 6.2.

Note that, according to the convention in 6.1, we have to use finally the index set $0, 1, 2$ instead of $1, 2, 3$. This final step of the procedure is here omitted.
In our opinion, the result just obtained is rather impressive because the partition of Ω^2 into the 2-orbits of the relatively large permutation group $Aut(\Gamma)$ is obtained by a purely combinatorial procedure based on "local" information about the symmetry of the graph Γ. We shall return to this example later.

6.11. Let $\mathcal{W}_1$ and $\mathcal{W}_2$ be cellular algebras of order n, and let $\mathcal{W}_1 \subseteq \mathcal{W}_2$. Then $\mathcal{W}_1$ is called a *cellular subalgebra* of $\mathcal{W}_2$.

Let $A \in M_n(\mathbb{C})$ be arbitrary. The minimal cellular algebra which contains A as an element is called the *cellular algebra generated by* A and will be denoted by $<< A >>$. This definition makes sense since due to Proposition 6.9 the intersection of cellular algebras is again a cellular algebra and $<< A >>$ can be thought as the intersection of all cellular subalgebras of $M_n(\mathbb{C})$ which contain A. The set $\mathcal{C}(A)$ of all such subalgebras is non-empty, because $M_n(\mathbb{C}) = \mathcal{V}_{\mathbb{C}}(\{e\}, \{1, 2, \ldots, n\}) \in \mathcal{C}(A)$. Since the set of all cellular algebras of a given order n is finite, the set $\mathcal{C}(A)$ is finite. Hence,

$$<< A >> = \bigcap_{\mathcal{W} \in \mathcal{C}(A)} \mathcal{W}$$

indeed determines a unique cellular algebra.

At the moment we do not want to introduce and discuss algorithms for constructing $<< A >>$ for any given matrix A. There is such an algorithm which is well-known as Weisfeiler-Leman stabilization (WL-stabilization for short), see [WeiL68], [Wei76]. A careful discussion of this stabilization procedure will be the subject of a forthcoming paper in our series. Here we will only demonstrate some examples where $<< A >>$ can be found using certain tricks mainly based on the Schur - Wielandt principle.[1]

6.12. Example:
Let Γ be the graph in Figure 6.3 and let $A = A(\Gamma)$ be its adjacency matrix. Find $\mathcal{W} = << A >>$.

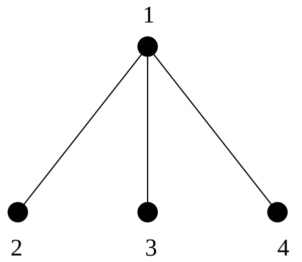


Figure 6.3.

We have

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

[1]The definition of $<< A >>$ can be interpreted to include validity of axiom (CA4) or not. Here we always assume that (CA4) is satisfied.

In the same manner as for a single matrix A a cellular algebra $<< A_1, A_2, \ldots, A_k >>$ generated by matrices $A_1, A_2, \ldots, A_k$ is defined. Clearly, if the matrices $A_1, A_2, \ldots, A_r$ form a standard basis of $\mathcal{W}$, then $<< A_1, A_2, \ldots, A_r >> = < A_1, A_2, \ldots, A_r > = \mathcal{W}$.

All we know at the beginning is that $A, I_4, J_4 \in << A >>$. Since $<< A >>$ is a vector space also

$$\bar{A} = J_4 - I_4 - A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

must belong to $<< A >>$. Now, since $<< A >>$ is closed with respect to matrix multiplication also

$$A^2 = \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix} \quad \text{and} \quad \bar{A}^2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 1 & 1 \\ 0 & 1 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{pmatrix}$$

are members of $<< A >>$. Applying the Schur - Wielandt principle we find the following two elements of $<< A >>$:

$$B_1 = \frac{1}{3} Y_3(A^2) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad B_2 = \frac{1}{2} Y_2(\bar{A}^2) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Redefining $B_3 = A$, $B_4 = \bar{A}$ we get a set of four $(0,1)$-matrices B_1, B_2, B_3 and B_4 with mutually disjoint support which sum up to J_4. However, this set is still not a basis for $<< A >>$, since $<< A >>$ has to contain products $B_i B_j$ and $B_j B_i$ for all $i, j = 1, 2, 3, 4$. In particular,

$$B_1 B_3 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad B_3 B_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

have to be members of $<< A >>$, resulting in a "desymmetrization" of the matrix A. This gives a new set of five matrices

$C_1 = B_1$,
$C_2 = B_2$,
$C_3 = B_1 A$,
$C_4 = A B_1$,
$C_5 = B_4$,

which is the desired basis for $<< A >>$. Indeed, all matrix products of the form $C_i C_j$ are in $< C_1, \ldots, C_5 >$ as can be seen from the following table of products:

	C_1	C_2	C_3	C_4	C_5
C_1	C_1	O	C_3	O	O
C_2	O	C_2	O	C_4	C_5
C_3	O	C_1	O	$3\,C_1$	$2\,C_3$
C_4	C_4	O	$C_2 + C_5$	O	O
C_5	O	C_5	O	$2\,C_4$	$2\,C_2 + C_5$

This proves already that $<C_1,\dots,C_5>$ is a matrix algebra in the usual sense. Moreover, the C_i have mutually disjoint support. Thus $<C_1,\dots,C_5>$ is closed with respect to S-H-multiplication. Since $C_1^t = C_1$, $C_2^t = C_2$, $C_3^t = C_4$, $C_4^t = C_3$, $C_5^t = C_5$ this space is also closed with respect to taking the transpose. Finally, $J_4 = C_1+C_2+C_3+C_4+C_5$. Therefore, $< C_1,\dots,C_5 >$ is a cellular algebra. By construction, $A \in\, < C_1,\dots,C_5 > \subseteq\, << A >>$. Hence, $< C_1,\dots,C_5 > = << A >>$. We have also $I_4 = C_1 + C_2 \in\, << A >>$.

This simple example was inserted in order to demonstrate that application of the Schur–Wielandt principle can simplify the computations for finding $<< A >>$. Moreover, the example shows that $<< A >>$ may contain antisymmetric basis elements even if A itself is a symmetric matrix. Indeed, in our case the subset of all symmetrical matrices from $<< A >>$ does not form a cellular algebra. As we shall see in one of the next papers one of the advantages of the WL-stabilization is that from the beginning this procedure automatically performs steps equivalent to "desymmetrization" and application of the Schur–Wielandt principle, thus reducing the number of necessary iterations.

6.13. Let $\mathcal{W} = < A_1, A_2, \dots, A_r >$ and $\mathcal{W}' = < B_1, B_2, \dots, B_s >$ be cellular algebras of order n. Let $\mathcal{W}'$ be a cellular subalgebra of $\mathcal{W}$. In this case $s \le r$, and there exists a partition $\mathcal{Q} = \{Q_1, Q_2, \dots, Q_s\}$ of the set $\{1, 2, \dots, r\}$ such that

$$B_j = \sum_{i \in Q_j} A_i$$

for all $j \in \{1, 2, \dots, s\}$.

For a given cellular algebra $\mathcal{W}$ and a cellular subalgebra $\mathcal{W}'$ the partition $\mathcal{Q}$ will be called the *basis partition*. A *"naive" approach* to the description of all cellular subalgebras of a given cellular algebra $\mathcal{W}$ (see [FarK91], [FarKM94]) is based on a preliminary selection of subsets of $\{1, 2, \dots, r\}$ (so-called *"good" subsets*) which satisfy certain necessary conditions to be a member of a basis partition. Then all possible partitions of $\{1, 2, \dots, r\}$ consisting of "good" subsets only are produced and examined. A program implementation COCO of this approach which was realized in [FarK91] shows good efficiency for cellular algebras of rank up to 30.

6.14. A cellular algebra $\mathcal{W} =< A_0, A_1, \dots, A_d >$ is called *commutative* if the matrix multiplication in $\mathcal{W}$ is commutative, i.e. if for all $A, B \in \mathcal{W}$ we have $AB = BA$. It is easy to see that if all basis matrices A_i, $0 \le i \le d$, are symmetric then $\mathcal{W}$ is commutative.

6.15. EXAMPLE:
Let Q_3 be the graph of the 3-dimensional cube which is depicted in Figure 6.4. It is well-known (see e.g. [KliPR88]) that $Aut(Q_3) \simeq S_4 \times S_2$, where $S_4 \times S_2$ is the direct product of the symmetric groups of degrees 4 and 2, $|S_4 \times S_2| = 48$.[1] Every automorphism of Q_3 has an interpretation as rotation or reflection of the 3-dimensional space, such that in case of Q_3 the sets of "geometrical" and of "combinatorial" symmetries coincide.

[1] $\simeq$ is the sign for the isomorphism of groups, see [Hal69], [Bis73].

Let $\Omega = \{0,1,2,3,4,5,6,7\}$, $G = Aut(Q_3)$, then $\mathit{2\text{-}orb}(G,\Omega) = \{R_0, R_1, R_2, R_3\}$ where for two vertices $x, y \in \Omega$ the pair $(x,y) \in R_i$ iff $d(x,y) = i$. Here $d(x,y)$ is the distance between x and y in the natural metric of the graph Q_3, i.e. the length of the shortest path between x and y.

We find $\mathcal{W}_0 = \mathcal{V}_{\mathbb{C}}(G,\Omega) = < A_0, A_1, A_2, A_3 >$ where $A_i = A(\Gamma_i)$, $\Gamma_i = (\Omega, R_i)$, $i \in \{0,1,2,3\}$. In particular, $\Gamma_1 = Q_3$. One can easily check the following part of the multiplication table for the commutative centralizer algebra W_0 (the trivial information on the matrix $A_0 = I_8$ is omitted):

$$\begin{aligned} A_1^2 &= 3\,A_0 + 2\,A_2, \\ A_1 A_2 &= 2\,A_1 + 3\,A_3, \\ A_1 A_3 &= A_2, \\ A_2^2 &= 3\,A_0 + 2\,A_2, \\ A_2 A_3 &= A_1, \\ A_3^2 &= A_0. \end{aligned}$$

Let us examine all three non-trivial partitions of $\{1,2,3\}$ as candidates for basis partitions of cellular subalgebras of $\mathcal{W}_0$. Let $\mathcal{W}_1 = <A_0, A_1, A_2 + A_3>$. This subspace does not form a subring because A_1^2 cannot be represented as linear combination of A_0, A_1 and $A_2 + A_3$.

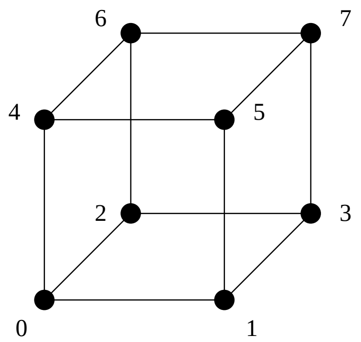


Figure 6.4.

Let $\mathcal{W}_2 = <A_0, A_1 + A_3, A_2>$. Here every test is successful, including

$$\begin{aligned} (A_1 + A_3)^2 &= 4\,A_0 + 4\,A_2, \\ (A_1 + A_3)\,A_2 &= 3\,A_1 + 3\,A_3. \end{aligned}$$

This means that $\mathcal{W}_2$ is a cellular subalgebra of $\mathcal{W}_0$. In the same manner we check that $\mathcal{W}_3 = < A_0, A_1 + A_2, A_3 >$ is a cellular subalgebra of $\mathcal{W}_0$. Altogether there are exactly 4 cellular subalgebras of $\mathcal{W}_0$:

$\mathcal{W}_0$, $\mathcal{W}_2$, $\mathcal{W}_3$ and $\mathcal{W}_4 = < A_0, A_1 + A_2 + A_3 >$.

The subalgebras $\mathcal{W}_0$ and $\mathcal{W}_4$ are called *trivial* or *improper* subalgebras.[1]

[1]For commutative cellular algebras $\mathcal{W}$ there is a more efficient method for finding all cellular subalgebras which is based on a certain duality theorem which involves spectral properties of the matrices in $\mathcal{W}$

7 Galois correspondence between permutation groups and cellular algebras

7.1. Let $\Gamma = (\Omega, R)$ be a graph with adjacency matrix A. The cellular algebra $<<A>>$ generated by A is also called the cellular algebra *generated by* Γ, or more simply, just the cellular algebra *of* Γ. Sometimes we shall denote it also by $\mathcal{W}(\Gamma)$. In this notation no reference is made to A.

In this section we want to discuss how one can find $Aut(\Gamma)$ if $\mathcal{W}(\Gamma)$ is known. In general, $\mathcal{W}(\Gamma)$ does not allow to determine $Aut(\Gamma)$ efficiently, i.e. with only a few computational steps. However, there are many favorable cases where the knowledge of $\mathcal{W}(\Gamma)$ leads more or less immediatly to $Aut(\Gamma)$. In particular, this is the case when $\mathcal{W}(\Gamma)$ contains the adjacency matrices of other graphs the automorphism group of which is known or is easier to determine, or when $\mathcal{W}(\Gamma)$ is even generated by one or more of such graphs. Note that $\mathcal{W}(\Gamma)$ may have many different generators. In order to be able to exploit the information given by $\mathcal{W}(\Gamma)$ exhaustively we must be able to compare cellular algebras and to find alternative generators, and sometimes we must even simultanously look at cellular algebras which are not generated by a single graph but only by two or even more graphs.

7.2. Let us start with a very simple case. Given an undirected graph $\Gamma = (\Omega, R)$ its *complementary* graph $\bar{\Gamma} = (\Omega, \bar{R})$ is defined by the complementary edge set

$$\bar{R} = \{\, \{x, y\} \,:\, x \neq y \wedge \{x, y\} \notin R\,\},$$

i.e. $\bar{\Gamma}$ is loopless and has an edge exactly where Γ has no edge. To have an example look at Figure 7.1. The right part of this figure, consisting of two components, is the complementary graph of the connected graph on the left side. Instead of complementary graph we say also shortly the *complement* of Γ.

If A is the adjacency matrix of Γ then we get the adjacency matrix $\bar{A}$ of $\bar{\Gamma}$ by exchanging 0 and 1 in the non-diagonal positions of A. More precisely, assuming $|\Omega| = n$, we have $\bar{A} = J_n - I_n - A$. This shows that $\bar{A} \in <<A>>$. Clearly, $\bar{\bar{A}} = A$.

It follows from the definition of an automorphism that $Aut(\Gamma) = Aut(\bar{\Gamma})$. Since $\bar{A} \in \mathcal{W}(\Gamma)$, we have $\mathcal{W}(\bar{\Gamma}) \subseteq \mathcal{W}(\Gamma)$. Since $A \in \mathcal{W}(\bar{\Gamma})$, also $\mathcal{W}(\Gamma) \subseteq \mathcal{W}(\bar{\Gamma})$ is true. Hence, $\mathcal{W}(\Gamma) = \mathcal{W}(\bar{\Gamma})$, i.e. A and $\bar{A}$ are different generating elements of $\mathcal{W}(\Gamma)$.

It may happen that replacing a graph Γ by its complement $\bar{\Gamma}$ will simplify the task of determining $Aut(\Gamma)$ substantially. We are going to illustrate this by the next two examples.

and the so-called second standard basis (see e.g. [BanI84]). The discussion of this method lies beyond the purpose of this paper. For the main criterion for the existence of a cellular subalgebra in a given commutative cell, the *Bannai–Muzychuk criterion*, we refer to the papers [Ban91] and [FarKM94].

7.3. Example:
Let Γ be the graph in the left part of of Figure 7.1. Find $Aut(\Gamma)$.

Γ is a regular graph of valency 4 with 7 vertices. $\bar{\Gamma}$ is also a regular graph of smaller valency 2. It is depicted in the right part of Figure 7.1. Evidently, $\bar{\Gamma} = C_3 \cup C_4$. (Remember that C_n denotes the undirected cycle on n vertices.)

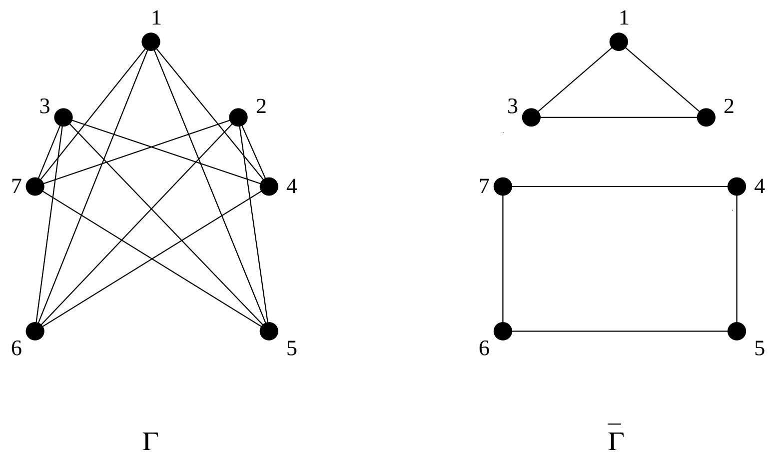


Figure 7.1.

In 4.32 we have found that $Aut(C_n) = D_n$, the dihedral group of order $2n$, acting as a transitive permutation group of degree n. (Note that the notation is different from the traditional notation in chemistry or crystallography). $\bar{\Gamma}$ consists of two non-isomorphic connected components. We may therefore apply Proposition 4.28 with the result that

$$Aut(\Gamma) = Aut(\bar{\Gamma}) = D_3 + D_4.$$

Hence, $Aut(\Gamma)$ is an intransitive permutation group of degree 7 and order 48.

7.4 Example:
Let Γ be the graph in Figure 7.2. Find $Aut(\Gamma)$.

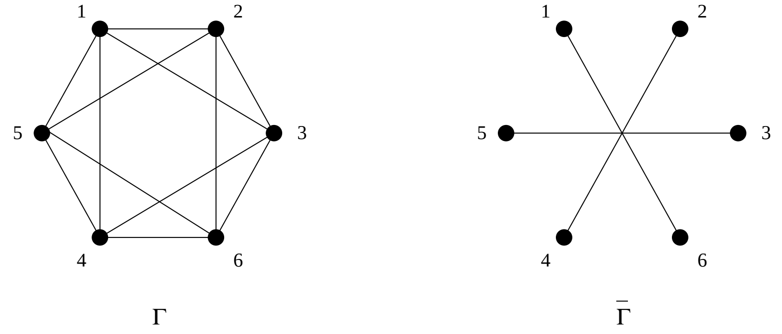


Figure 7.2.

Here the complement $\bar{\Gamma}$ is a disjoint union of edges. Hence, we may use Proposition 4.30 in order to find $Aut(\bar{\Gamma})$. Thus,

$$Aut(\Gamma) = Aut(\bar{\Gamma}) = S_3 \wr S_2.$$

This is a transitive permutation group of degree 6 and order 48.

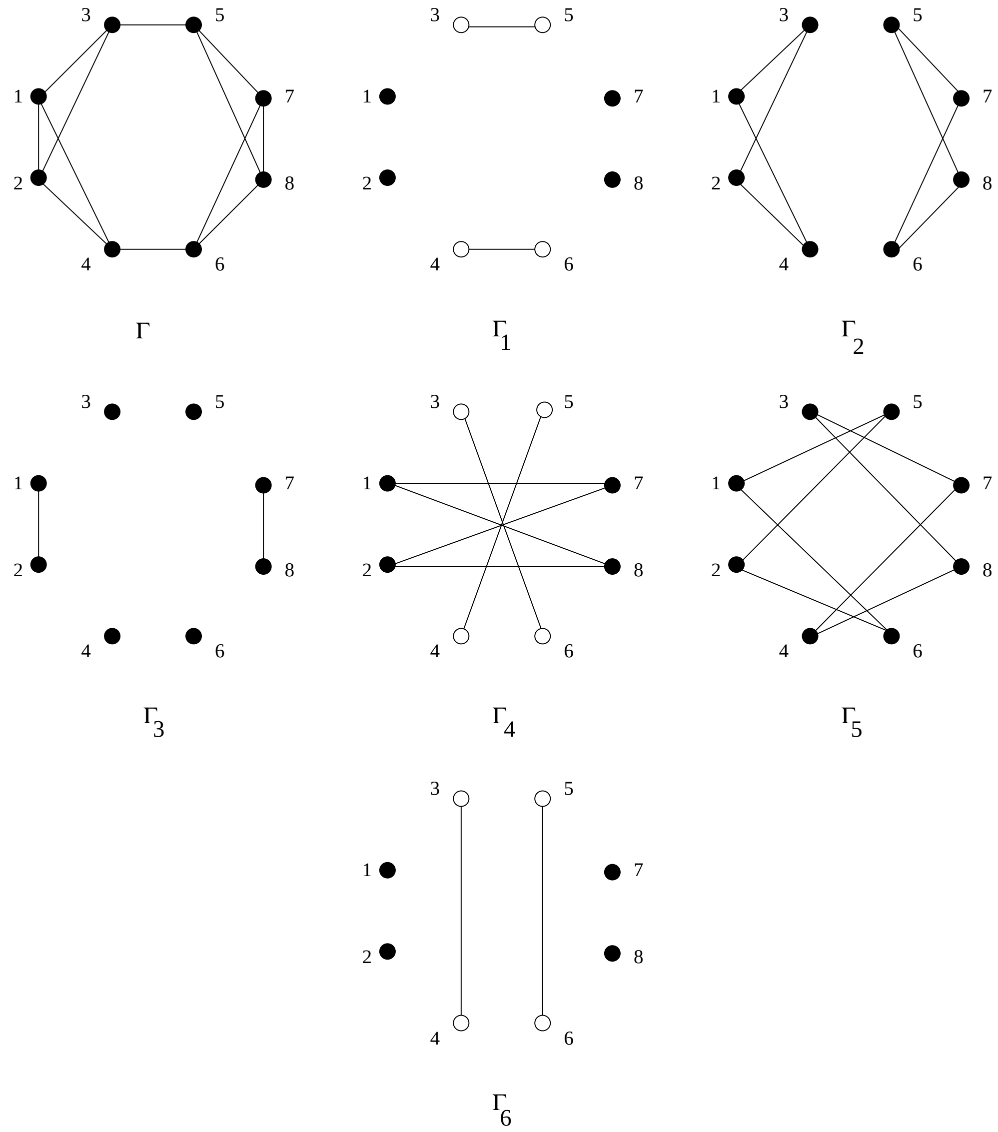


Figure 7.3

7.5. EXAMPLE:
Let $\Gamma = (\Omega, R)$ be the cubic graph shown as graph Γ_9 in Figure 2.3 and let $G = Aut(\Gamma)$ be its automorphism group. We would like to describe (G, Ω) in its action on the vertex set $\Omega = \{1, 2, 3, 4, 5, 6, 7, 8\}$ of Γ. We can do this conveniently by using some information available from the cellular algebra $\mathcal{W} = \mathcal{W}(\Gamma)$ generated by Γ.

Let us classify the edges (x, y) of Γ according to the number of joint neighbors of the endpoints x and y in Γ. We get

$$R_1 = \{(x, y) \in R : \ x \text{ and } y \text{ have no joint neighbor } \},$$

$$R_2 = \{(x, y) \in R : \ x \text{ and } y \text{ have exactly one joint neighbor } \},$$
$$R_3 = \{(x, y) \in R : \ x \text{ and } y \text{ have exactly two joint neighbors } \}.$$

The same classification for non-edges of Γ gives three more relations

$$R_4 = \{(x, y) \notin R \ : \ x \text{ and } y \text{ have no joint neighbor } \},$$

$$R_5 = \{(x, y) \notin R : \ x \text{ and } y \text{ have exactly one joint neighbor } \},$$
$$R_6 = \{(x, y) \notin R : \ x \text{ and } y \text{ have exactly two joint neighbor } \}.$$

Each relation $R_1, R_2, \ldots, R_6$ is a symmetric binary relation on Ω. Let $\Gamma_i = (\Omega, R_i)$ be the graph with vertex set Ω and edge set R_i, $1 \leq i \leq 6$, and let $A_i = A(\Gamma_i)$ and $A = A(\Gamma)$ be the adjacency matrices of Γ_i and Γ, respectively. In subsection 7.6 we shall prove that $A_i \in \mathcal{W}$. The graphs Γ and Γ_i, $1 \leq i \leq 6$ are depicted in Figure 7.3.

In Figure 7.3 some automorphisms of Γ are immediately visible as "geometric" symmetries of Γ, for instance, $g_1 = (1,7)(2,8)(3,5)(4,6)$ and $g_2 = (1,2)(3,4)(5,6)(7,8)$. It is easy to check that $g_1 g_2 = g_2 g_1$. Thus $G' =< g_1, g_2 >= \{e, g_1, g_2, g_1 g_2\}$, is a group of order 4, and $G' \leq G$.

Each automorphism of Γ evidently has to preserve each of the relations $R_1, \ldots, R_6$. Therefore, $G \leq \bar{G}$, where $\bar{G} = \bigcap_{i=1}^{6} Aut(\Gamma_i)$. For this reason we temporarily will aim at a new goal: to find the permutation group $(\bar{G}, \Omega)$. After that we will try to discover the group (G, Ω) itself. Considering Γ_1, for example, we see that $Aut(\Gamma_1)$, and hence $\bar{G}$, preserves the subsets $\Omega' = \{1, 2, 7, 8\}$ and $\Omega'' = \{3, 4, 5, 6\}$. Taking into account that already G' acts transitively on Ω' and Ω'' we get that Ω' and Ω'' are orbits of $(\bar{G}, \Omega)$.

Consider the subgraphs of $\Gamma_1, \Gamma_4, \Gamma_6$ which are generated by the subset Ω''. To find these subgraphs easily, in Figure 7.3 the vertices of Ω'' in these graphs are marked by empty circles. Since $\bar{G}$ has to preserve these subgraphs, the action of $\bar{G}$ on Ω'' may include only permutations from the permutation group (H'', Ω'') where

$$H'' = \{e'', (3,4)(5,6), (3,5)(4,6), (3,6)(4,5)\}$$

(compare with Example 5.11).

In the same manner we see that the action of $\bar{G}$ on Ω' may include only permutations of (H', Ω') where $H' =< (1,2), (7,8), (1,7)(2,8) >$. (H' is a group of order 8 which is isomorphic to the dihedral group D_4.)

Combining the above two informations we get that $\bar{G} \leq H = H' + H''$. H is an intransitive permutation group of order $4 \cdot 8 = 32$ acting on Ω.

On the next step of our reasoning we observe that in fact $h'' = (3,5)(4,6) \in H''$ is not an automorphism of Γ_2 (more exactly, $e' + h'' = (1)(2)(3,5)(4,6)(7)(8)$ does not belong to $Aut(\Gamma_2)$). Therefore, $\bar{G}$ is a proper subgroup of H. This implies $|H : \bar{G}| > 1$, such that due to the Lagrange Theorem (see 4.2) we get $|\bar{G}| \leq 16$.

Just now we are rather close to the description of the desired group G. The remaining part we do by counting arguments. Consider the permutations

$$h_1 = (1,2), \quad h_2 = (7,8), \quad h_3 = (3,4)(5,6), \quad h_4 = (1,8)(2,7)(3,5)(4,6).$$

It is easily checked that all of them are automorphisms of Γ. Hence,

$$\hat{G} = < h_1, h_2, h_3, h_4 > \leq G.$$

Further, $< h_1, h_2, h_3 >$ is a group of order 8 which does not contain h_4, hence, by the same argument as before, we have $|\hat{G}| \geq 16$. Now together with $|\bar{G}| \leq 16$, since $\hat{G} \leq G \leq \bar{G}$, we have $|\hat{G}| = |G| = |\bar{G}| = 16$. Therefore $\hat{G} = G = \bar{G}$. Thus, G is a permutation group of order 16, which acts transitively on each of the sets Ω' and Ω''.

7.6. *Cellular Expressibility*
Let us have another look onto the strategy which was used in Example 7.5 in order to get the automorphism group G of a given graph Γ. We started with the relation R which describes the edge set of Γ. From R we derived more and different relations $R_1, \ldots, R_6$ which are preserved by every automorphism of Γ. The corresponding adjacency matrices $A_1, \ldots, A_6$ belong to $\mathcal{W}$. We suggest the reader to check that all of them can be obtained from A by means of the operations introduced in Section 6. Indeed,

$$\begin{aligned} A_1 &= Y(0, A^2) \circ A, \\ A_2 &= Y(1, A^2) \circ A, \\ A_3 &= Y(2, A^2) \circ A, \\ A_4 &= Y(0, A^2) \circ \bar{A}, \\ A_5 &= Y(1, A^2) \circ \bar{A}, \\ A_6 &= Y(2, A^2) \circ \bar{A}. \end{aligned}$$

In a case like this, when $A_i \in << A >>$, we say that the matrices A_i, $1 \leq i \leq$, are *cellularly expressible* via the matrix A. Likewise we say that the graphs $\Gamma_i = (\Omega, R_i)$ are *cellularly expressible* via the graph Γ.

Cellular expressibility of graphs Γ_i, $i \in \{1, \ldots, s\}$ via a graph Γ implies that each automorphism of Γ is also an automorphism of each of the Γ_i, i.e.

$$Aut(\Gamma) \subseteq \bigcap_{i=1}^{s} Aut(\Gamma_i).$$

Suppose that we are able to show that also Γ is cellularly expressible via Γ_i, $1 \le i \le s$, which means that $A \in << A_1, \dots, A_s >>$. Then each joint automorphism of the Γ_i's is also an automorphism of Γ, and therefore

$$\bigcap_{i=1}^{s} Aut(\Gamma_i) \subseteq Aut(\Gamma).$$

In this case we finally get

$$Aut(\Gamma) = \bigcap_{i=1}^{s} Aut(\Gamma_i).$$

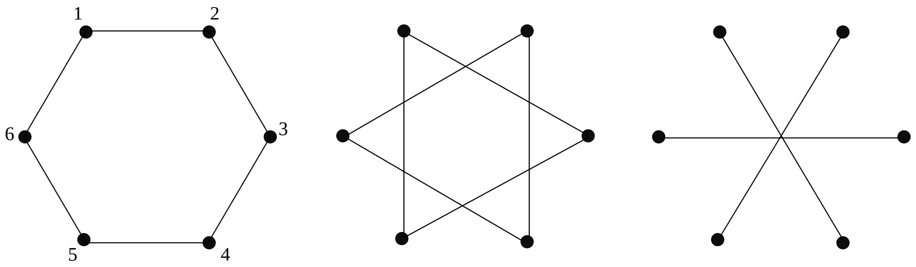
This situation happens in the above example, where $A = A_1 + A_2 + A_3$. Hence, we could have known in advance that in fact $G = \bar{G}$. The analysis of the group $\bar{G}$ is therefore sufficient for getting the desired group G. This observation motivates the definition of the automorphism group of a cellular algebra which is given in the next subsection.

7.7. To every cellular algebra $\mathcal{W} = < A_1, A_2, \dots, A_r >$ we associate its *automorphism group* $Aut(\mathcal{W})$ which acts on the set $\Omega = \{1, 2, \dots, n\}$. We define

$$Aut(\mathcal{W}) = \bigcap_{i=1}^{r} Aut(R_i),$$

where $\{R_1, R_2, \dots, R_r\}$ is the set of basic relations (see 6.8) of $\mathcal{W}$.

According to this definition, an automorphism of $\mathcal{W}$ is a permutation of Ω which preserves all the basic relations, i.e. g is an automorphism of $\mathcal{W}$ if and only if g is an automorphism of each basis graph $\Gamma_i = (\Omega, R_i)$, $1 \le i \le r$. Therefore, it is evident that $Aut(\mathcal{W}) \subseteq Aut(\Gamma_i)$. It may happen that equality holds in some of these inclusions, i.e. that $Aut(\mathcal{W}) = Aut(\Gamma_i)$ for some Γ_i. It may happen also that the inclusion is strict for all basic graphs Γ_i. Let us illustrate this fact by looking at some simple examples.



S $\quad$ S' $\quad$ S''

Figure 7.4

7.8 EXAMPLE:
Consider the undirected cycle C_6 in Figure 7.4. This is an undirected graph consisting of the vertex set $\Omega = \{1, 2, 3, 4, 5, 6\}$ and the symmetric relation $S = R \cup R^t$ where

$$R = \{(1, 2), (2, 3), (3, 4), (4, 5), (5, 6), (6, 1)\}.$$

Let P denote the adjacency matrix of the graph (Ω, R). Then, evidently, the adjacency matrix of C_6 is $A = A(C_6) = P + P^t$. Consider also the symmetric relations S' and S'' in Figure 7.4. It is easy to find by inspection, that each of them is invariant with respect to D_6, the automorphism group of C_6. Just remember that this group consists of 6 rotations and 6 reflections (discussed in 4.31 and 4.32). The adjacency matrices of S' and S'' are

$$B = A(S') = P^2 + (P^t)^2, \; C = A(S'') = P^3 + (P^t)^3.$$

Using this and the fact that $PP^t = P^6 = I_6$, we can easily check the following "table of products":

	I	A	B	C
I	I	A	B	C
A	A	2I+B	A+2C	B
B	B	A+2C	2I+B	A
C	C	B	A	I

Here the letter I stands for I_6. Note that I is the adjacency matrix of the identity relation id_Ω on the set Ω.

We have $I + A + B + C = J_6$. No two of the matrices I, A, B and C have a joint positive entry. According to the above table the product of any two of them is a linear combination of I, A, B and C. This proves that $\{I, A, B, C\}$ is the standard basis of some cellular algebra $\mathcal{W}$ (see 6.1). Since $A \in \mathcal{W}$, we have $\mathcal{W}(A) \subseteq \mathcal{W}$. However, $B = A^2 - 2I$ and $C = A^3 - 3A$. This implies $B \in \mathcal{W}(A)$ and $C \in \mathcal{W}(A)$. Therefore, $\mathcal{W} \subseteq \mathcal{W}(A)$. Hence, $\mathcal{W} = \mathcal{W}(A)$ and id_Ω, S, S', S'' are the basic relations of the cellular algebra $\mathcal{W}$, which is generated by A.

We have,

$$Aut(id_\Omega) = S_6, \; Aut(S) = D_6, \; Aut(S') \supseteq D_6, \; Aut(S'') \supseteq D_6.$$

Therefore,

$$Aut(\mathcal{W}) = Aut(id_\Omega) \cap Aut(S) \cap Aut(S') \cap Aut(S'') = Aut(S) = D_6.$$

The relation S' is invariant with respect to $g' = (1)(2)(3,5)(4,6)$, the relation S'' is invariant with respect to $g'' = (1,4)(2,5)(3)(6)$. Neither g' nor g'' belongs to D_6. Hence, we have the strict inclusions $Aut(\mathcal{W}) \subset Aut(S')$ and $Aut(\mathcal{W}) \subset Aut(S'')$.

7.9 EXAMPLE:
Let us look again at Example 5.11 which was started already in 4.9. Consider Figure 5.4. In the upper part of this figure 4 graphs Γ_i, $1 \le i \le 4$, on the vertex set $\Omega = \{1, 2, 3, 4\}$ are depicted. Assume that $\Gamma_i = (\Omega, R_i)$, where the relations R_1, R_2, R_3, R_4, which are the 2-orbits of the group G in 4.9, are numbered in the same order as they appear in the figure. Their adjacency matrices $A_i = A(R_i)$ are

$$A_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \; A_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \; A_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \; A_4 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

Hence, $\mathcal{V}(G,\Omega) =< A_1, A_2, A_3, A_4 >$, and the four relations R_1, R_2, R_3, R_4 are the basic relations of this cellular algebra, the centralizer algebra of G acting on Ω.

We see immediately that $A_i^2 = I_4$, $1 \leq i \leq 4$. Further, denoting by $\bar{A}_i$ the adjacency matrix of the complement of (Ω, R_i), we have

$$\bar{A}_1 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}, \; \bar{A}_2 = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}, \; \bar{A}_3 = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}, \; \bar{A}_4 = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}.$$

A simple computation gives

$$\bar{A}_2^2 = 2I_4 + 2A_2, \;\; A_2\bar{A}_2 = \bar{A}_2 A_2 = \bar{A}_2.$$

Therefore, the cellular algebra $<< A_2 >>$ generated by A_2 has standard basis $I_4, A_2, \bar{A}_2$, and is therefore a strict subalgebra of $\mathcal{V}(G,\Omega)$. A similar computation easily shows that $<< A_3 >>$ has standard basis $I_4, A_3, \bar{A}_3$, and $<< A_4 >>$ has standard basis $I_4, A_4, \bar{A}_4$. We therefore have to conclude that $\mathcal{V}(G,\Omega)$ is not generated by a single basis graph Γ_i. However, some more simple computation would demonstrate that any two of the graphs $\Gamma_2, \Gamma_3, \Gamma_4$ do the job, i.e.

$$\mathcal{V}_{\mathbb{C}}(G,\Omega) = << A_2, A_3 >> = << A_2, A_4 >> = << A_3, A_4 >> .$$

Evidently, $Aut(\Gamma_1) = S_4$, $Aut(\Gamma_i) \supset G$ for $i = 2, 3, 4$. The groups $Aut(\Gamma_i)$, $i = 2, 3, 4$, are isomorphic. However, their action on Ω is different. We have

$$(Aut(\Gamma_2), \Omega) = \{e, (1,2), (1,2)(3,4), (3,4), (1,3)(2,4), (1,4)(2,3), (1,3,2,4), (1,4,2,3)\},$$

$$(Aut(\Gamma_3), \Omega) = \{e, (1,2)(3,4), (1,3), (1,3)(2,4), (2,4), (1,4)(2,3), (1,2,3,4), (1,4,3,2)\},$$

$$(Aut(\Gamma_4), \Omega) = \{e, (2,3), (1,2)(3,4), (1,3)(2,4), (1,4), (1,4)(2,3), (1,2,4,3), (1,3,4,2)\}.$$

This shows that

$$\bigcap_{i=1}^{4} Aut(\Gamma_i, \Omega) = \bigcap_{i=2}^{4} Aut(\Gamma_i, \Omega) = \{e, (1,2)(3,4), (1,4)(2,3), (1,3)(2,4)\} = G.$$

7.10 The two foregoing examples differ in one crucial point:

In Example 7.8 the cellular algebra $\mathcal{W}$ is generated by a single graph $\Gamma = (\Omega, S)$ (which, by the way, is a basic graph). The two other basic graphs $\Gamma' = (\Omega, S')$ and $\Gamma'' = (\Omega, S'')$ are cellularly expressible via Γ. The automorphism group of $\mathcal{W}$ is (therefore) identical with the automorphism group of Γ.

In Example 7.9 $\mathcal{W}$ is not generated by a single graph. It is generated only by two graphs out of $\{\Gamma_2, \Gamma_3, \Gamma_4\}$. Hence, the automorphism group of $\mathcal{W}$ is the intersection of any two of the groups $Aut(\Gamma_1), Aut(\Gamma_2), Aut(\Gamma_3)$, i.e.

$$Aut(\mathcal{W}) = Aut(\Gamma_1) \cap Aut(\Gamma_2) = Aut(\Gamma_1) \cap Aut(\Gamma_3) = Aut(\Gamma_2) \cap Aut(\Gamma_3.$$

One can easily prove that if $\mathcal{W}$ is generated by a set of graphs $\{\Gamma_1, \ldots, \Gamma_r\}$ then

$$Aut(\mathcal{W}) = \bigcap_{i=1}^{r} Aut(\Gamma_i).$$

7.11 At this point we want once more, and now very decidedly, to call the readers attention that in this and in the previous sections we kept talking about two very particular types of objects - "categories" of objects one would say to use a philosophical term. On one hand we consider *cellular algebras*, these are collections of matrices, namely the adjacency matrices of certain binary relations and their linear combinations over the field $\mathbb{C}$. We think of these adjacency matrices as *representatives* of combinatorial objects, i.e. graphs, molecules, etc. On the other hand we consider *permutation groups,* the elements of which make the symmetries of combinatorial objects evident. So we speak of "combinatorial objects" and their "symmetries".

For each relation R there is a group of automorphisms, i.e. a group of permutations which leave R unchanged. For each permutation g there is a set of relations which are left unchanged by g, i.e. for which g is an automorphism.

In Section 5 we started with a permutation group (G, Ω) and looked for the set of all relations R with $Aut(R) = G$. We found that we may represent any such relation as a union of certain basic relations invariant under G. These basic relations were called 2-orbits of (G, Ω). After representing them by adjacency matrices and taking their linear combinations with arbitrary coefficients from $\mathbb{C}$ we ended up with the notion of the centralizer algebra $\mathcal{V}(G, \Omega)$, which turned out to be a cellular algebra. Hence, for each permutation group (G, Ω) there is a corresponding cellular algebra $\mathcal{V}(G, \Omega)$.

In Section 6 we introduced the notion of a cellular algebra $\mathcal{W}$, which is an algebra of matrices the basic matrices of which correspond to a set of binary relations on a set Ω. These relations we call the basic relations of $\mathcal{W}$. Therefore, in Subsection 7.7, we naturally came to the definition of the automorphism group of $\mathcal{W}$ as the group of permutations of Ω which leave all basic relations invariant. Hence, for every cellular algebra $\mathcal{W}$ on Ω there is a corresponding group of permutations of Ω, the automorphism group $Aut(\mathcal{W})$.

In fact we have two mappings

$$\mathcal{W} \longrightarrow Aut(\mathcal{W}),$$

$$G \longrightarrow \mathcal{V}(G,\Omega),$$

one (denoted as *Aut*) which leads from a cellular algebra $\mathcal{W}$ to its automorphism group $Aut(\mathcal{W})$, and one (denoted as $\mathcal{V}$) which leads from a permutation group (G,Ω) to its centralizer algebra $\mathcal{V}(G,\Omega)$.

It is good to know the automorphism group $Aut(\mathcal{W})$ of a cellular algebra $\mathcal{W}$, because knowing this group means to have quite a deal of information about the symmetry of the relations which are encoded by the matrices of $\mathcal{W}$. It is good to know the centralizer algebra $\mathcal{V}(G,\Omega)$ of a permutation group (G,Ω), because knowing this cellular algebra means to have quite a lot of information about the action of (G,Ω) on the set Ω^2.

Our goal is now to manipulate skillfully with the above two mappings *Aut* and $\mathcal{V}$. We may think of the world in which we work as divided into two working places. On one of them we work with cellular algebras, on the other place we work with permutation groups. We may start with a cellular algebra $\mathcal{W}$ on one place and move to the other place to find $(G,\Omega) = (Aut(\mathcal{W}),\Omega)$. Having found this group perhaps we have forgotten where we came from and may in turn ask which cellular algebra has (G,Ω) as its group of automorphisms. So we may go back again to the first working place and find $\mathcal{V}(G,\Omega) = \mathcal{V}(Aut(\mathcal{W}),\Omega)$. Naturally, we will ask "Is $\mathcal{V}(G,\Omega) = \mathcal{W}$? The answer is "Very often, but not always." Similarly, we may start with a permutation group (G,Ω) and move to its centralizer algebra $\mathcal{V}(G,\Omega)$. Having found this cellular algebra we may ask "What is its automorphism group ? Is it the group (G,Ω) ? " Again, the answer is "Very often, but not always."

For our goal, the description of the symmetries of combinatorial objects, those cases are the most important ones, in which the above questions are to be answered with "Yes". We will explain this carefully in the following subsections.

7.12. We start our explanations with a collection of statements which describe the most important features of the two mappings *Aut* and $\mathcal{V}$ considered in the last subsection. In this and in the following two subsections we shall assume that the set $\Omega = \{1,2,\ldots,n\}$ is fixed. All groups we are talking about will be permutation groups acting on Ω. All cellular algebras which appear in the discussion are supposed to be of order n. To simplify the notation, we shall write G instead of (G,Ω), however, we shall keep thinking of G as a permutation group acting on Ω.

Proposition. *Let $\mathcal{W}_1, \mathcal{W}_2$ be two cellular algebras of order n, and let G, H be permutation groups acting on $\Omega = \{1,2,\ldots,n\}$. Then:*

(i) $\mathcal{W}_1 \subseteq \mathcal{W}_2 \Longrightarrow Aut(\mathcal{W}_2) \leq Aut(\mathcal{W}_1)$;

(ii) $H \leq G \Longrightarrow \mathcal{V}(G) \subseteq \mathcal{V}(H)$;

(iii) $G \leq Aut(\mathcal{V}(G))$;

Moreover, for every cellular algebra $\mathcal{W}$ we have

(iv) $\mathcal{W} \subseteq \mathcal{V}(Aut(\mathcal{W}))$;

(v) $\mathcal{W} = \mathcal{V}(Aut(\mathcal{W})) \Longleftrightarrow \mathcal{W}$ *is the centralizer algebra of a suitable permutation group;*

(vi) $G = Aut(\mathcal{V}(G)) \Longleftrightarrow G^{(2)} = G$.

7.13 The first statement of the above Proposition can be proved very easily. Let $g \in Aut(\mathcal{W}_2)$. $\mathcal{W}_1 \subseteq \mathcal{W}_2$ means that every basic relation of $\mathcal{W}_1$ is a union of certain basic relations of $\mathcal{W}_2$. Since g leaves the basic relations of $\mathcal{W}_2$ invariant, it leaves also all unions of them invariant. Hence g is an automorphism of each basic relation of $\mathcal{W}_1$. Therefore, $g \in Aut(\mathcal{W}_1)$. This proves $Aut(\mathcal{W}_2) \subseteq Aut(\mathcal{W}_1)$.

The second statement is proved similarly. By definition, the basic relations of $\mathcal{V}(H)$ are the 2-orbits of H, while the basic relations of $\mathcal{V}(G)$ are the 2-orbits of G. Each 2-orbit of G is a relation which is invariant with respect to H. Hence, it is a union of 2-orbits of H. This shows that the basic relations of $\mathcal{V}(G)$ are unions of the basic relations of $\mathcal{V}(H)$, which means that $\mathcal{V}(G) \subseteq \mathcal{V}(H)$.

In general, when we move between working places forth and back according to the above mappings Aut and $\mathcal{V}$, then the following inclusions hold. If we start with $\mathcal{W}$ an one side, then

$$\mathcal{V}(Aut(\mathcal{W})) \supseteq \mathcal{W}.$$

This is clear, because, by definition, the basic relations of $\mathcal{V}(Aut(\mathcal{W}))$ are the 2-orbits of $Aut(\mathcal{W})$, and since the basis relations of $\mathcal{W}$ are invariant with respect to $Aut(\mathcal{W})$, they are unions of these 2-orbits. Hence, $\mathcal{W} \subseteq \mathcal{V}(Aut(\mathcal{W}))$ ((*iii*) of Proposition 7.12). However, in general, $\mathcal{W}$ does not contain every union of 2-orbits of $Aut(\mathcal{W})$. Therfore, it may happen, that $\mathcal{W}$ has less elements than $\mathcal{V}(Aut(\mathcal{W}))$ (see 7.16 for an example).

Similarly, if we start with G on the other side, then

$$Aut(\mathcal{V}(G)) \supseteq G.$$

This is also clear, since the basic relations of $\mathcal{V}(G)$ are the 2-orbits of G. Therefore they are invariant with respect to G. Thus, every $g \in G$ is an automorphism of $\mathcal{V}(G)$ ((*iv*) of Proposition 7.12). However, in general, there can be additional automorphism of $\mathcal{V}(G)$ which do not belong to G (see 7.15 for an example).

Now, assume that $\mathcal{W} = \mathcal{V}(Aut(\mathcal{W}))$ for some cellular algebra $\mathcal{W}$. Then $\mathcal{W}$ is the centralizer algebra of the group $Aut(\mathcal{W})$. Hence, assume that $\mathcal{W} = \mathcal{V}(G)$ for some permutation group G. Then the basic relations of $\mathcal{W}$ are the 2-orbits of G which implies that $G \leq Aut(\mathcal{W})$. The 2-orbits of any overgroup of G are unions of 2-orbits of G. Hence, the basic relations of $\mathcal{V}(Aut(\mathcal{W}))$ are unions of 2-orbits of G, which means that $\mathcal{V}(Aut(\mathcal{W})) \subseteq \mathcal{V}(G) = \mathcal{W}$. Together with statement (*iv*) this gives $\mathcal{W} = \mathcal{V}(Aut(\mathcal{W}))$.

Similarly, if $G = Aut(\mathcal{V}(G))$ for some permutation group G, then there is no permutation of Ω outside G which preserves all the 2-orbits of G, i.e. the basic relations of $\mathcal{V}(G)$. This means, that no strict overgroup of G has the same 2-orbits as G. By definition, this is the case if and only if $G = G^{(2)}$ (see 5.12).

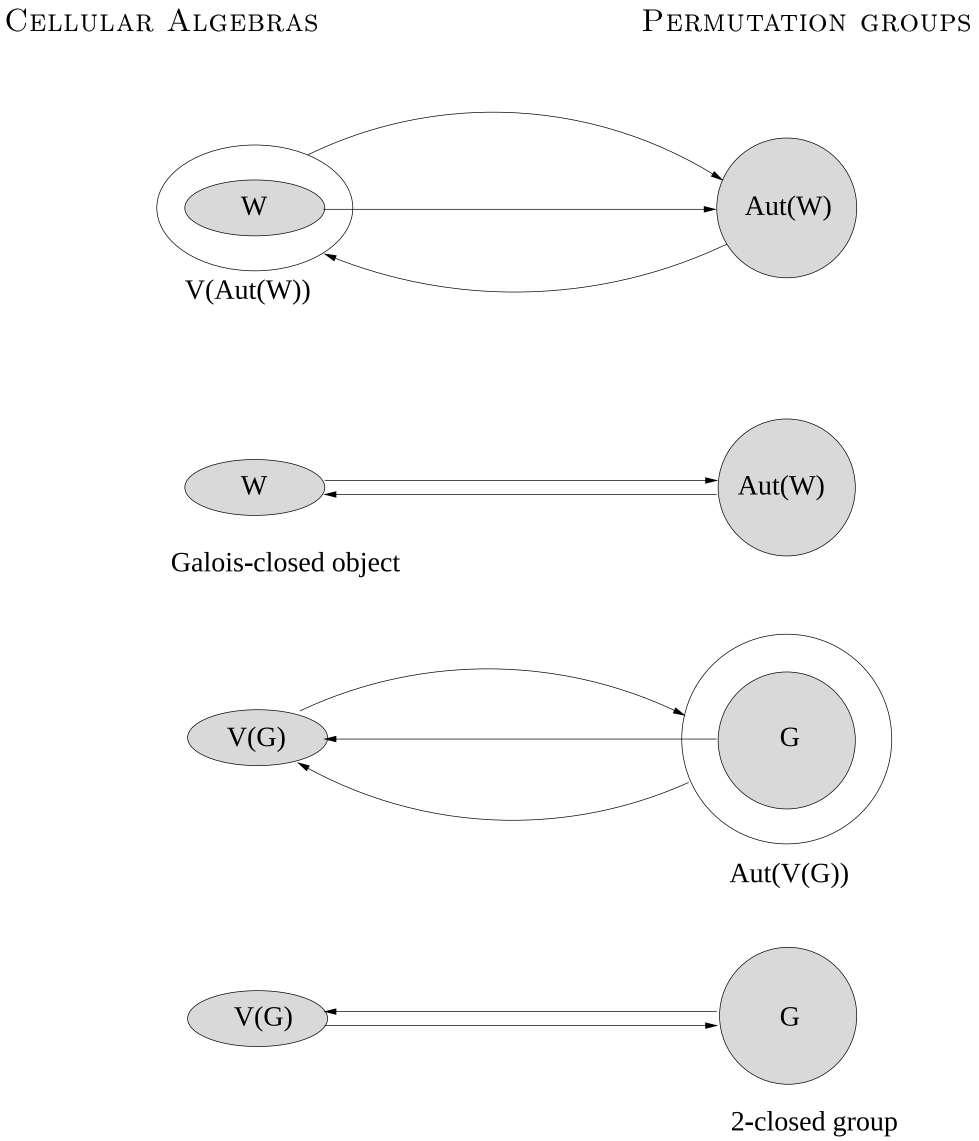


Figure 7.5

7.14. The mappings *Aut* and $\mathcal{V}$ which we have considered in the last subsections are called *Galois correspondences* (between the two types of objects, namely cellular algebras and permutation groups). Cellular algebras $\mathcal{W}$ which fulfill $\mathcal{W} = \mathcal{V}(Aut(\mathcal{W}))$ and permutation groups G which fulfill $G = Aut(\mathcal{V}(G))$ are called *Galois-closed objects*. Clearly, for permutation groups Galois-closed means the same as 2-closed. A Galois-closed cellular algebra is also called a *Schurian* cellular algebra.

Figure 7.5 illustrates what happens when we change our working place several times. The first picture explains that we can get larger cellular algebras, if we start with a cellular algebra, compute its automorphism group, and then compute the centralizer algebra of this group. The second picture explains the case when a cellular algebra is Schurian. The third and the fourth pictures explain the analoguous cases which appear when we start with a permutation group, compute its centralizer algebra, and then compute the automorphism group of this algebra.

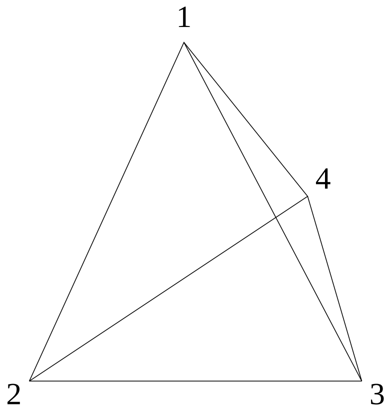


Figure 7.6

7.15. Let us consider a simple example of the fact that $Aut(\mathcal{V}(G,\Omega))$ is strictly larger than (G,Ω). Consider the symmetric group S_4 acting on $\Omega_4 = \{1,2,3,4\}$ and its subgroup

$$(Alt_4,\Omega_4) = \{e,(1)(2,4,3),(1)(2,3,4),(1,3,4)(2),$$
$$(1,4,3)(2),(1,2,4)(3),(1,4,2)(3),(1,2,3)(4),$$
$$(1,3,2)(4),(1,2)(3,4),(1,3)(2,4),(1,4)(2,3)\},$$

consisting of 12 permutations which can be considered as the group of rotations of a regular tetrahedron (see Figure 7.6.)

The 2-orbits of (Alt_4,Ω_4) are

$$R_1 = \{(1,1),(2,2),(3,3),(4,4)\}, \quad R_2 = \Omega_4 \times \Omega_4 - R_1.$$

However, these are also the 2-orbits of (S_4,Ω_4). Hence, $(Alt_4,\Omega_4) \neq (Alt_4^{(2)},\Omega_4) = (S_4,\Omega_4)$.

The example given here is only one member of an infinite series of examples. Let $g \in (Alt_4,\Omega_4)$ be given. A pair $(i,j), i,j \in \Omega$ is called an *inversion* of g, if $i < j$ and $i^g > j^g$ holds. The reader may convince himself by investigation that (Alt_4,Ω_4) consists exactly of all permutations g in (S_4,Ω_4) which have an even number of inversions.

Consider (S_n,Ω_n), where $n \in \boldsymbol{N}, n \geq 4$, is arbitrary and $\Omega_n = \{1,2,\ldots,n\}$. The subset (Alt_n,Ω_n) of (S_n,Ω_n) consisting of all permutations in (S_n,Ω_n) which have an even number of inversions is a subgroup of S_n. This subgroup is called the *alternating group* of permutations of Ω_n, whence the notation Alt_n (cf 5.15). One can show that its 2-orbits are

$$R_1 = \{(1,1),\ldots,(n,n)\} \text{ (the } \textit{diagonal} \text{ of } \Omega_n \times \Omega_n),$$
$$R_2 = \Omega_n \times \Omega_n - R_1.$$

Again, these are also the 2-orbits of (S_n,Ω_n). Thus we have $(Alt_n,\Omega_n) \neq (Alt_n^{(2)},\Omega_n) = (S_n,\Omega_n)$ for every natural number $n > 3$. However, $(Alt_3,\Omega_3) = (Alt_3^{(2)},\Omega_3)$. Thus, the example with $n = 4$ we started with is just the first one in an infinite series of examples of groups which are not 2-closed.

7.16. Next we shall demonstrate by an example that graphs can exist, the cellular algebra of which (in contrast to naive expectation) does not fully reflect the true symmetry.

Consider a so-called Latin square Σ, which is an $n \times n$ table the n^2 cells of which are occupied by n copies of the numbers $0,1,2,\ldots,n-1$. Repetition of a number within a row or within a column is not allowed. An example for $n = 4$ is given in Figure 7.7a.

0	1	2	3
1	2	3	0
2	3	0	1
3	0	1	2

a)

0	1	2	3
4	5	6	7
8	9	10	11
12	13	14	15

b)

Figure 7.7

Let us construct the graph $\Gamma(\Sigma)$ of this Latin square as follows: Vertices of the graph are the 16 cells of the square, labelled sequentially as in Figure 7.7b. An edge is drawn between any two vertices that are either in the same row, or in the same column, or are occupied by the same number in Σ. Thus in our example vertex 0 is connected by an edge to vertices $1, 2, 3, 4, 7, 8, 10, 12, 13$. The adjacency matrix of Γ can be easily written, though the corresponding diagram looks somewhat complicated.

In order to get a nicer diagram, we now consider the complementary graph to the above, $\bar{\Gamma}(\Sigma)$, which is called the *Shrikhande graph* and denoted by Sh. Sh has edges where Γ has non-edges and vice versa, e.g. vertex 0 is connected to vertices $5, 6, 9, 11, 14, 15$. Sh is still a nonplanar graph, but it can be drawn without crossing of edges on the surface of a torus. The plane diagram of Sh given in Figure 7.8 with vertex labels is to be understood such that the vertices situated on the periphery of the solid-line figure are further connected as indicated by dotted lines.

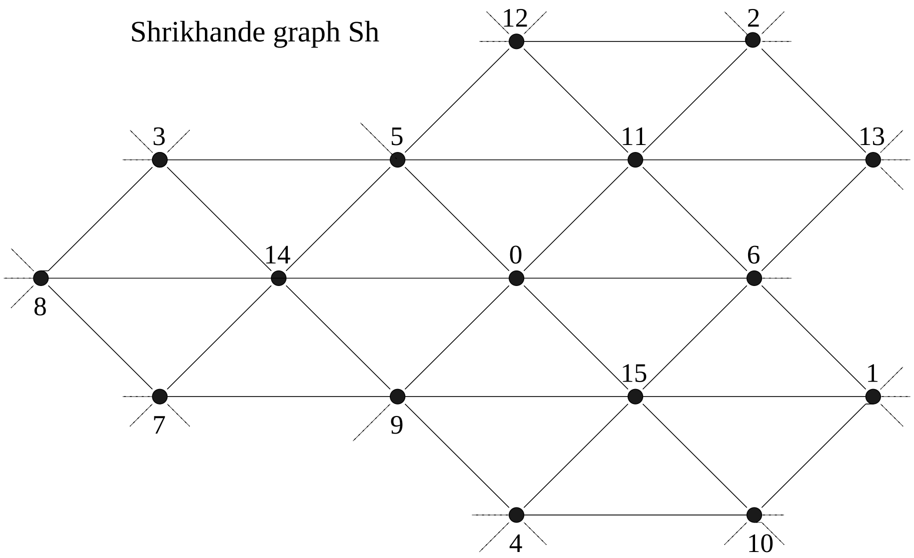


Figure 7.8.

The full information about the connections in Sh is given by the adjacency matrix $\bar{A} = A(Sh)$ which is

$$\bar{A} = \begin{pmatrix}
0&0&0&0&0&1&1&0&0&1&0&1&0&0&1&1\\
0&0&0&0&0&0&1&1&1&0&1&0&1&0&0&1\\
0&0&0&0&1&0&0&1&0&1&0&1&1&1&0&0\\
0&0&0&0&1&1&0&0&1&0&1&0&0&1&1&0\\
0&0&1&1&0&0&0&0&0&1&1&0&0&1&0&1\\
1&0&0&1&0&0&0&0&0&0&1&1&1&0&1&0\\
1&1&0&0&0&0&0&0&1&0&0&1&0&1&0&1\\
0&1&1&0&0&0&0&0&1&1&0&0&1&0&1&0\\
0&1&0&1&0&0&1&1&0&0&0&0&0&1&1&0\\
1&0&1&0&1&0&0&1&0&0&0&0&0&0&1&1\\
0&1&0&1&1&1&0&0&0&0&0&0&1&0&0&1\\
1&0&1&0&0&1&1&0&0&0&0&0&1&1&0&0\\
0&1&1&0&0&1&0&1&0&0&1&1&0&0&0&0\\
0&0&1&1&1&0&1&0&1&0&0&1&0&0&0&0\\
1&0&0&1&0&1&0&1&1&1&0&0&0&0&0&0\\
1&1&0&0&1&0&1&0&0&1&1&0&0&0&0&0
\end{pmatrix}.$$

The following observations on Γ are easily made by inspection of Figure 7.7.

- Γ is a regular graph of valency 9.
- For each edge of Γ the number of neighbors common to its vertices is the same, namely 4. For example, vertices 0 and 1 (connected by an edge) have 2, 3, 4 13 as common neighbors.
- For each non-edge of Γ the number of neighbors common to its vertices is the same, namely 6. For example, vertices 0 and 5 (not connected by an edge) have 1, 2, 4, 7, 8, 13 as common neighbors.

Corresponding statements are valid for Sh, as seen by inspection of Figure 7.8 and of the adjacency matrix $\bar{A}$. It is a regular graph of valency 6, the number of neighbors common to the vertices of any edge is 2, and the number of neighbors common to any two non-connected vertices is also 2.

Now it is easy to show that Γ generates a cellular algebra of rank 3. For this purpose, a few matrix products are calculated. Let $A = A(\Gamma)$ be the adjacency matrix of Γ, then $\bar{A} = A(Sh) = J - I - A$. A^2 and $\bar{A}^2$ are easily obtained by using a well-known result of graph theory: The entries in the square of an adjacency matrix are the numbers of walks of length 2, that is, the numbers of neighbors common to two connected or non-connected vertices in the respective graph (see [Har69], compare Section 5.26):

$$A^2 = 9I + 4A + 6\bar{A},$$

$$\bar{A}^2 = 6I + 2A + 2\bar{A}.$$

Further,

$$A\bar{A} = A(J - I - A) = AJ - AI - A^2 = 9J - A - (9I + 4A + 6\bar{A})$$

$$= 9(I + A + \bar{A}) - A - (9I + 4A + 6\bar{A}) = 4A + 3\bar{A}.$$

Finally, we can see that

$$A\bar{A} = \bar{A}A.$$

Thus, all products of the matrices $I, A, \bar{A}$ are linear combinations of these matrices, and therefore $\mathcal{W} =< I, A, \bar{A} >=<< \Gamma >>=<< Sh >>$ is a matrix algebra (see 5.19). Moreover, it is a cellular algebra of rank 3 (see axioms in Section 6.1). In other words, $\mathcal{W}$ is the cellular algebra generated by Γ. We have obviously $Aut(\mathcal{W}) = Aut(\Gamma)$.

Now the question arises whether $\mathcal{W}$ is Galois-closed, in other words, whether the equation $\mathcal{W} = \mathcal{V}(Aut(\mathcal{W}))$ is true. If it is, then $G = Aut(\Gamma)$ has exactly three 2-orbits: one (described by I) for vertices, another one (described by A) for edges, and the last one (described by $\bar{A}$) for non-edges. In particular, all edges are equivalent in this case, which means that all edges should have identical values for each possible numerical edge characteristic.

A useful characteristic of an edge is the number α of 4-vertex complete subgraphs (4-cliques) in which this edge is involved. Let us determine α of edge $\{0, 1\}$ and of edge $\{0, 10\}$ in Γ. These numbers are easily read from Figure 7.9a and 7.9b, respectively. There the labeling scheme of vertices is the same as in Figure 7.7b, and the numbers given are those from Figure 7.7a (the numbers by which the cells of the Latin square are occupied). A 4-clique involving edge $\{0, 1\}$ is found whenever two common neighbors of 0 and 1 are connected by an edge. Common neighbors of 0 and 1 are $2, 3, 4, 13$, and of these only 2 and 3 are connected by an edge. Hence, $\alpha(\{0, 1\}) = 1$. Common neighbors of 0 and 10 are $2, 7, 8, 13$, and of these both 2 and 8 and 7 and 13 are connected by edges, which means that $\alpha(\{0, 10\}) = 2$.

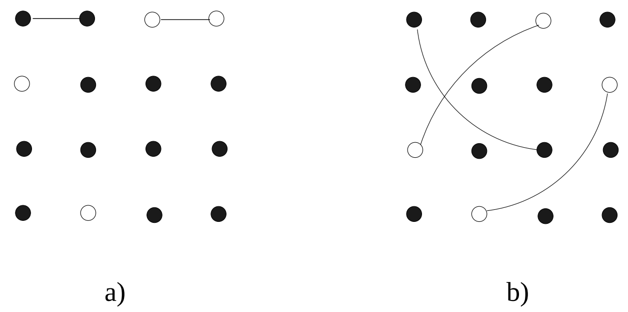


Figure 7.9.

Therefore, there are at least two different types of edges in Γ, the cellular algebra $\mathcal{W}$ does not adequately describe the symmetry of Γ, and thus $\mathcal{W}$ is not Galois-closed, i.e. $\mathcal{V}(Aut(\mathcal{W}))$ has more basic relations than $\mathcal{W}$.

8 S-rings over cyclic groups

8.1. *(Arithmetic operations modulo n).* Let n be a natural number and consider the cycle $(0, 1, \ldots, n-1)$. Its graph is shown in Figure 8.1 (with $n = 16$).

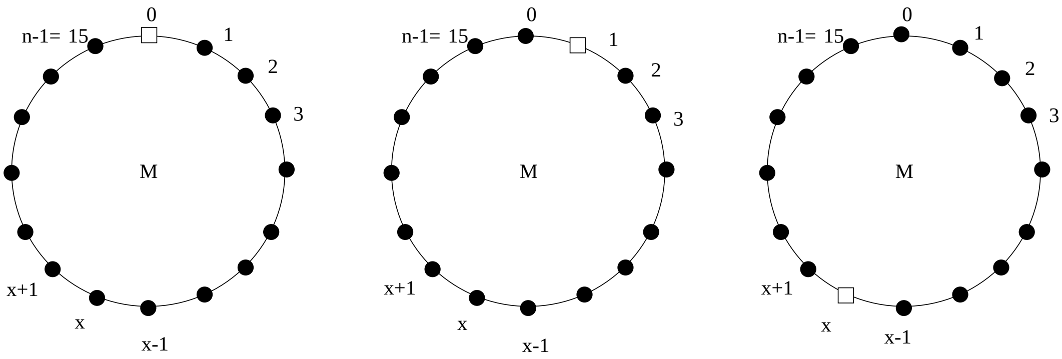


Figure 8.1

If we let the cycle rotate clockwise around an axis through the center M and perpendicular to the plane, then the small square which is currently in position 0 will wander clockwise step by step into position $1, 2, \ldots$, and after performing x steps it will be situated in position x. Each single step corresponds to a rotation by the angle $\frac{2\pi}{n}$.

Now, what will be the position of the square after a sequence of x steps followed by a sequence of y steps ? If $x + y < n$, then the position will be just $x + y$. If $x + y = n$, then the position will be 0, the square has made a full cycle and has reached its start position again. If $x + y > n$, then, clearly, the square has started a second time and has reached position $x + y - n$. This observation leads us to the definition of a certain operation on the set $\boldsymbol{Z}$, which is usually called *addition of integers modulo n.* The operator symbol is $\oplus$, it is defined by

$$x \oplus y = \begin{cases} x + y & \text{if } 0 \leq x + y < n \\ x + y - \lfloor \frac{x+y}{n} \rfloor \cdot n & \text{if } \quad x + y \geq n \text{ or } x + y < 0, \end{cases}$$

where for any rational number z the notation $\lfloor z \rfloor$ means the largest integer less or equal to z. In a similar way, the *multiplication of integers modulo n* is defined.

We shall write $x \ominus y$ instead of $x \oplus (n - y)$. The operation $\ominus$ is inverse to $\oplus$.

If we restrict x and y to the set $\{0, 1, \ldots, n-1\}$, then $\oplus$ becomes an associative and commutative binary operation on this set, 0 acts as neutral element, and each element x has its inverse element, namely $-x = n - x$. Thus, $\{0, 1, \ldots, n-1\}$ is a commutative group under the operation $\oplus$, the *group of residue classes modulo n*, usually denoted by $\boldsymbol{Z}_n$.

For any $x \in \boldsymbol{Z}_n$ the element $-x$ can be interpreted as an anti-clockwise rotation of the cycle in Figure 8.1 by the angle $\frac{x \cdot 2\pi}{n}$ which brings the square, when being in position x, back to the start position 0. Note that, if we start the rotation anti-clockwise going as far as x steps, then we reach the same position as when we go clockwise as far as $n-x$ steps.

8.2. *(Cyclic groups).* Each $i \in \boldsymbol{Z}_n$ defines a permutation of $\boldsymbol{Z}_n$ which maps $x \in \boldsymbol{Z}_n$ onto $x \oplus i$. For instance, if $n = 7$ and $i = 3$, we get the permutation $(0, 3, 6, 2, 5, 1, 4)$ of $\boldsymbol{Z}_7 = \{0, 1, 2, 3, 4, 5, 6\}$. For $n = 12$ and $i = 4$ we get the permutation $(0, 4, 8)(1, 5, 9)(2, 6, 10)(3, 7, 11)$ of $\boldsymbol{Z}_{12} = \{0, 1, \ldots, 10, 11\}$.

Let π be the permutation of $\boldsymbol{Z}_n$ which is defined using $i = 1$, i.e.

$$x^\pi = x \oplus 1,\ x \in \boldsymbol{Z}_n.$$

It generates a group $<\pi>$ the elements of which are the powers π^i of π, where the action of π^i on $\boldsymbol{Z}_n$ is equal to the i-fold application of π, i.e.

$$\begin{array}{rcl} x^{\pi^2} & = & (x^\pi)^\pi = (x \oplus 1) \oplus 1 = x \oplus 2 \\ x^{\pi^3} & = & ((x^\pi)^\pi)^\pi = (x \oplus 2) \oplus 1 = x \oplus 3 \\ & \ldots & \end{array}$$

and in general,

$$x^{\pi^i} = x \oplus i,$$

for which reason we introduce the notation

$$\pi_i = \pi^i.$$

In particular, $\pi_1 = \pi$ and $\pi_n = e$, the neutral element. Further

$$<\pi_1> = \{e, \pi_1, \pi_2, \ldots, \pi_{n-1}\}.$$

A group which is generated by a single element is called a *cyclic group.*

Evidently, $(<\pi_1>, \boldsymbol{Z}_n)$ is a transitive permutation group of order n and degree n. Transitive permutation groups of order equal to the degree are called *regular* groups. Since the elements of $<\pi_1>$ are in 1-to-1 correspondence with the elements of $\boldsymbol{Z}_n$, we use for $<\pi_1>$ also the notation $\boldsymbol{Z}_n$ (thus π_i identifying with $i \in \boldsymbol{Z}_n$). In particular we shall consider the pair $(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$, where the group $\boldsymbol{Z}_n$ is considered to act on itself via the shifts

$$x \longmapsto x \oplus i,\ x \in \boldsymbol{Z}_n.$$

This is the *action* of $i \in \boldsymbol{Z}_n$ *on* $\boldsymbol{Z}_n$.

8.3. Consider once more a cycle like in Figure 8.1, however, this time with directed edges, such that we get a directed graph with vertex set $V = \boldsymbol{Z}_n$ and arc set $\Phi_1 = \{\,(x, x \oplus 1) : x \in \boldsymbol{Z}_n\,\}$. Its adjacency matrix is (for n = 6 as an example)

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Now, each power P^i of P is also a permutation matrix and defines an arc set (a binary relation) $\Phi_i = \{\,(x, x \oplus i) : x \in \boldsymbol{Z}_n\,\}$ on $\boldsymbol{Z}_n$. Figure 8.2 shows the six different graphs $\Gamma_i = (\boldsymbol{Z}_6, \Phi_i)$, $0 \le i \le 5$.

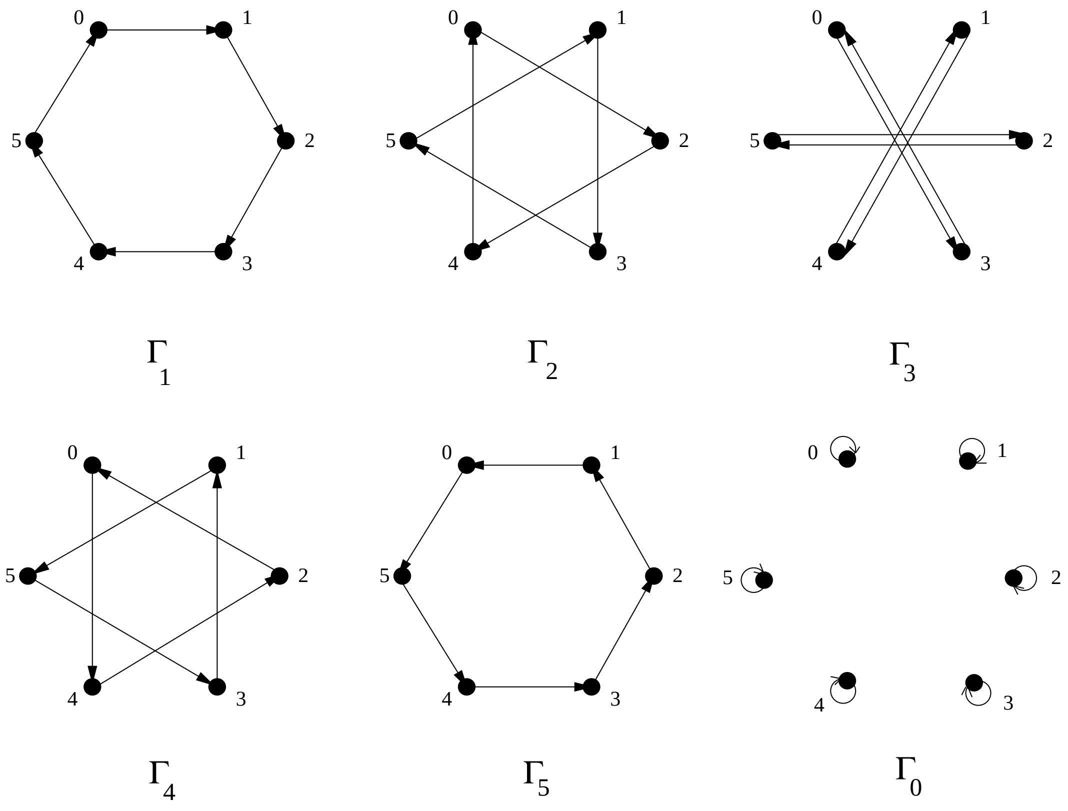


Figure 8.2.

In general, i.e. for $n \in \boldsymbol{N}$ arbitrary, P^i is a matrix representation of the permutation π_i of $\boldsymbol{Z}_n$. Thus we have three different representations for one and the same object. π_i is a *mapping* from $\boldsymbol{Z}_n$ onto $\boldsymbol{Z}_n$, $i \in \boldsymbol{Z}_n$ is just a *number* the knowledge of which allows to perform the mapping π_i via the formula $x^{\pi^i} = x \oplus i$. Finally, P^i is a *permutation matrix* of order n which again by its non-zero entries determines the mapping π_i, i.e. $x^{\pi^i} = y$ if and only if $P^i_{x,y} = 1$. Accordingly, we have three different *representations* for the group $<\pi_1>$. The first representation is $<\pi_1>$ itself, where the group elements are mappings and the group operation is the *consecutive performing* of mappings. The second representation is

$\boldsymbol{Z}_n$, where the group elements are integers and the group operation is *addition modulo n.* The third representation is $< P >= \{ P^0, P^1, \ldots, P^{n-1} \}$, where the group elements are matrices and the group operation is *multiplication of matrices.* Clearly, $P^n = P^0 = I_n$, the identity matrix of order n.

All three representations are groups which are obviously isomorphic. Hence, all of them are cyclic groups. Since *addition modulo n* has more or less similar features like the usual addition of integers and since *multiplication of matrices* has similar features like the usual multiplication of numbers, we call $\boldsymbol{Z}_n$ a group in *additive notation* whereas $< P >$ and $<\pi_1>$ are said to be a group in *multiplicative notation.*

8.4. Each relation Φ_i on $\boldsymbol{Z}_n$ is invariant wih respect to $(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$. Moreover, each Φ_i is minimal with respect to this property, i.e. no strict subset of Φ_i is also an invariant relation. Hence,

$$\textit{2-orb}(\boldsymbol{Z}_n, \boldsymbol{Z}_n) = \{ \Phi_i \,:\, i \in \boldsymbol{Z}_n \}.$$

In the language of matrices, *invariance* of Φ_i means that its adjacency matrix P^i *commutes* with every power P^j of P, a trivial observation, since in fact, $P^i P^j = P^j P^i = P^{i \oplus j}$, which is equivalent to the equality $\pi_i \pi_j = \pi_{i \oplus j}$.

Again, assume for example $n = 6$. Figure 8.2 shows the graphs of the relations $\Phi_0, \ldots, \Phi_5$, which are the six elements in *2-orb*$(\boldsymbol{Z}_6, \boldsymbol{Z}_6)$. In addition, below all the corresponding 6 adjacency matrices are listed:

$$P^0 = \begin{pmatrix} 1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&1&0&0&0\\ 0&0&0&1&0&0\\ 0&0&0&0&1&0\\ 0&0&0&0&0&1 \end{pmatrix}, \quad P^1 = \begin{pmatrix} 0&1&0&0&0&0\\ 0&0&1&0&0&0\\ 0&0&0&1&0&0\\ 0&0&0&0&1&0\\ 0&0&0&0&0&1\\ 1&0&0&0&0&0 \end{pmatrix}, \quad P^2 = \begin{pmatrix} 0&0&1&0&0&0\\ 0&0&0&1&0&0\\ 0&0&0&0&1&0\\ 0&0&0&0&0&1\\ 1&0&0&0&0&0\\ 0&1&0&0&0&0 \end{pmatrix},$$

$$P^3 = \begin{pmatrix} 0&0&0&1&0&0\\ 0&0&0&0&1&0\\ 0&0&0&0&0&1\\ 1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&1&0&0&0 \end{pmatrix}, \quad P^4 = \begin{pmatrix} 0&0&0&0&1&0\\ 0&0&0&0&0&1\\ 1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&1&0&0&0\\ 0&0&0&1&0&0 \end{pmatrix}, \quad P^5 = \begin{pmatrix} 0&0&0&0&0&1\\ 1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&1&0&0&0\\ 0&0&0&1&0&0\\ 0&0&0&0&1&0 \end{pmatrix}.$$

Throughout this Section 8, P will denote the adjacency matrix of the cycle $\Gamma_1 = (\boldsymbol{Z}_n, \Phi_1)$. The order n of P will be clear from the context. Hence, P^i will be the adjacency matrix of $\Gamma_i = (\boldsymbol{Z}_n, \Phi_i)$. Note that according to our current notation the initial row (and column) of any P^i has index 0. Note once more that due to the definition of the Φ_i's each P^i is a permutation matrix, i.e. $P^i = M(\pi_i)$. Each row and each column of P^i contains exactly one entry equal to 1, all other entries being 0. More exactly,

$$(P^i)_{kj} = \begin{cases} 1 & \text{if} \quad j = k \oplus i \\ 0 & \text{otherwise.} \end{cases}$$

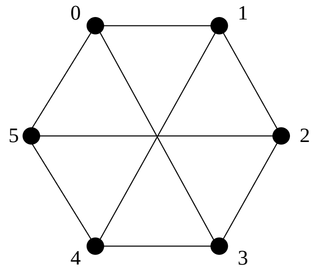
Since the relations Φ_i are the 2-orbits of $(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$ they are at the same time the basis relations of the centralizer ring (centralizer algebra) $\mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$. Hence, $\{P^0, P^1, \ldots, P^{n-1}\}$ is the standard basis of $\mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$.

8.5. *(Circulant graphs).* Now, having at hand the relations Φ_i, $0 \leq i \leq n-1$, let us combine some of them to get a new relation Φ on $\boldsymbol{Z}_n$ and let us consider it as the arc set of a new graph Γ. To be precise, for arbitrary $X \subseteq \boldsymbol{Z}_n$ define

$$\Phi = \Phi(X) = \bigcup_{k \in X} \Phi_k \text{ and } \Gamma(X) = (\boldsymbol{Z}_n, \Phi).$$

$\Gamma(X)$ is a graph with vertex set $\boldsymbol{Z}_n$ and arc set Φ which is invariant with respect to $(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$. Graphs Γ with this property are called *circulant graphs* or *cyclic graphs.* The set X is called the *connection set* of Γ. [1]

Figure 8.3 gives an example of a circulant graph on $\boldsymbol{Z}_6$ with $X = \{1, 3, 5\}$. Its adjacency matrix $A = A(\Gamma)$ reads



$$A = \begin{pmatrix} 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 \end{pmatrix} = P^1 + P^3 + P^5.$$

Figure 8.3.

In general, the adjacency matrix A of a circulant graph $\Gamma(X)$ is

$$A = A(X) = \sum_{k \in X} P^k.$$

It is a so-called *circulant matrix*, i.e. it has the property $a_{i \oplus l, j \oplus l} = a_{i,j}$ for any $l \in \boldsymbol{Z}_n$. On the other hand, if the adjacency matrix of a graph Γ is a circulant matrix $A = A(X)$, then Γ is a circulant graph with connection set X.

8.6. It follows from the definition that a graph $\Gamma = (\boldsymbol{Z}_n, \Phi)$ is a circulant graph if and only if its automorphism group $Aut(\Gamma)$ contains the group $(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$. In general, however, this automorphism group may be much larger than $(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$. Circulant graphs play an important role also in mathematical chemistry. In order to study the symmetries of such a graph we have to find its automorphism group, or at least to find the system of 2-orbits of this group. As we saw in previous chapters, the set of basis relations of the cellular

[1] If (H, H) is a regular permutation group and Γ is a graph which is invariant with respect to H (a condition which implies that H is the vertex set of Γ), then Γ is called *Cayley graph* over H. In the case considered here $H = \boldsymbol{Z}_n$. Thus, circulant graphs are Cayley graphs over $\boldsymbol{Z}_n$.

ring $<<A>>$ generated by the adjacency matrix A are unions of 2-orbits and, therefore, are invariant with respect to $(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$. In order to find the basis relations of $<<A>>$ we have to start with $A_1 = A, A_2 = I_n$ and $A_3 = J_n - I_n - A$, we have to compute their usual products and their S-H products in order to get more and more elements from $<<A>>$ until we end up with the standard basis of this cellular algebra (see Section 6 and 7). Each of the matrices involved is a certain weighted sum of powers of P. For instance,

$$A_1 = \sum_{k\in X} P^k, \quad A_2 = P^0, \quad A_3 = \sum_{k\in \boldsymbol{Z}_n - X - \{0\}} P^k.$$

Further, take $n = 7$ and $X = \{1, 4\}$ for example, then $A = A_1 = P^1 + P^4$, and

$$\begin{array}{rcl} A_1^2 & = & P^1 + P^2 + 2P^5, \\ A_1^3 & = & 3P^2 + P^3 + P^5 + 3P^6, \\ A_1^2 \circ A_1^3 & = & 3P^2 + 2P^5, \\ & \ldots & \end{array}$$

and so on. In general, assume

$$B = \sum_{k\in X_B} b_k P^k$$

with integers b_k and some subset X_B of $\boldsymbol{Z}_n$. If we define $b_k = 0$ for $k \notin X_B$, then we get

$$B = \sum_{k\in \boldsymbol{Z}_n} b_k P^k.$$

This is a polynomial in P of degree less than or equal to $n - 1$. Clearly, we know B if we know the vector $b = (b_0, b_1, \ldots, b_{n-1})$. Further, assume $c = (c_0, c_1, \ldots, c_{n-1})$ and $C = \sum_{k\in \boldsymbol{Z}_n} c_k P^k$. Then

$$B \circ C = \sum_{k\in \boldsymbol{Z}_n} b_k c_k P^k.$$

Thus the S-H product of B and C is defined by the vector of its coefficients, which in turn is found by multiplying b and c componentwise. But what is BC ? We have

$$BC = \sum_{k\in \boldsymbol{Z}_n} \sum_{l\in \boldsymbol{Z}_n} b_k c_l P^{k+l} = \sum_{j\in \boldsymbol{Z}_n} \Big(\sum_{k\oplus l = j} b_k c_l \Big) P^j.$$

Thus the coefficient β_j of P^j in the polynomial for BC is given by

$$\beta_j = \sum_{k\in \boldsymbol{Z}_n} b_k c_{j\ominus k}.$$

We see therefore, that multiplying two matrices B and C each of which is a polynomial in P with coefficient vectors b and c, respectively, can be done by performing some simple operations applied to b and c. This fact offers an option for an alternative and computationally much more convenient way to compute the cellular ring associated with a circulant graph Γ, or in fact, to compute a certain algebraic structure equivalent to this cellular ring which is called S-ring and which we are going now to discuss in the following subsections of this section.

8.7. Let $\boldsymbol{Z}(\boldsymbol{Z}_n)$ (this is new notation) denote the set of all *formal combinations* of elements of $\boldsymbol{Z}_n$ with integral coefficients, i.e. all *formal sums* of the form

$$\sum_{i \in \boldsymbol{Z}_n} \lambda_i \, i, \quad \lambda_i \in \boldsymbol{Z}.$$

Note the similarity of this expression with the polynomials considered in 8.4 which we get if we replace i by P^i. Note also that there is no multiplication sign '$\cdot$' between the coefficients λ_i and the number i at the right of them, i.e. you are not meant to multiply λ_i by i and sum up really. A formal sum is merely a different notation for a sequence of integers λ_i, i.e. for

$$(\lambda_0, \lambda_1, \lambda_2, \ldots, \lambda_{n-1}),$$

(which, for instance, can be used to build up a polynomial in P). When we want to operate in a particular way with objects of this kind the notation as formal sums is very convenient.

If $\lambda = \sum_{i \in \boldsymbol{Z}_n} \lambda_i \, i$ and $K = \{ i \, : \, \lambda_i \neq 0 \}$ then we shall write also $\lambda = \sum_{i \in K} \lambda_i \, i$.

Let us introduce the following operations on $\boldsymbol{Z}(\boldsymbol{Z}_n)$. Given

$$\lambda = \sum_{i \in \boldsymbol{Z}_n} \lambda_i \, i, \; \mu = \sum_{i \in \boldsymbol{Z}_n} \mu_i \, i$$

and given $\rho \in \boldsymbol{Z}$ we define

$$\begin{aligned}
\rho\lambda &= \sum_{i \in \boldsymbol{Z}_n} (\rho\lambda_i) \, i \\
\lambda + \mu &= \sum_{i \in \boldsymbol{Z}_n} (\lambda_i + \mu_i) \, i \\
\lambda \circ \mu &= \sum_{i \in \boldsymbol{Z}_n} (\lambda_i \mu_i) i \\
\lambda * \mu &= \sum_{i \in \boldsymbol{Z}_n} \sum_{j \in \boldsymbol{Z}_n} (\lambda_i \mu_j) \, i \oplus j = \sum_{i \in \boldsymbol{Z}_n} (\sum_{j \in \boldsymbol{Z}_n} \lambda_j \mu_{i \ominus j}) i.
\end{aligned}$$

Supplied with these operations, the set $\boldsymbol{Z}(\boldsymbol{Z}_n)$ is called *integer group ring* over $\boldsymbol{Z}_n$.

There are very special elements in $\boldsymbol{Z}(\boldsymbol{Z}_n)$ for which we want to have a slightly more simple notation. Assume $X \subset \boldsymbol{Z}_n$, $X = \{x_1, x_2, \ldots, x_r\}$. The formal sum $\sum_{i \in \boldsymbol{Z}_n} \lambda_i^X \, i$ where $\lambda_i^X = 1$ if $i \in X$ and $\lambda_i^X = 0$ if $i \notin X$ can be thought as a representative of the subset X. Therefore, we use also the notation

$$\underline{X} = \underline{x_1, x_2, \ldots, x_r} = \sum_{i \in \boldsymbol{Z}_n} \lambda_i^X \, i.$$

Formal sums of the form $\underline{X}$ are called *simple quantities* of $\boldsymbol{Z}(\boldsymbol{Z}_n)$. A simple quantity is a list in which every entry has multiplicity 1. If X is a set, then $\underline{X}$ is a list of the elements of X which can be subjected to the operations $+, \circ, *$ introduced above.

Simple quantities enable us to simplify calculations. First of all, a 1-element subset $\underline{i} = \{i\}$ of $\boldsymbol{Z}_n$ may be identified with i, hence in any formal sum $\sum_{i \in \boldsymbol{Z}_n} \lambda_i \, i$ the group elements i may be replaced by $\underline{i}$, i.e.

$$\sum_{i \in \boldsymbol{Z}_n} \lambda_i \, i = \sum_{i \in \boldsymbol{Z}_n} \lambda_i \underline{i}.$$

Now, for example, assume $n = 6$ and

$$\lambda = 3\,\underline{0} + 3\,\underline{1} + 2\,\underline{2} + 2\,\underline{3} + 3\,\underline{4} + 3\,\underline{5} =$$

$$= 3\,\underline{0,1,4,5} + 2\,\underline{2,3}.$$

The first expression for λ means that we have a list of elements of $\boldsymbol{Z}_6$, with multiple entries, where the elements 0, 1, 4 and 5 appear thrice, whereas 2 and 3 appear only twice, the second expression tells us that this list is made up by two different sublists $\{0,1,4,5\}$ and $\{2,3\}$, the first being used three times, the second only twice.

As seen in this example, the elements of $\boldsymbol{Z}(\boldsymbol{Z}_n)$ can be considered as lists of elements of $\boldsymbol{Z}_n$ with multiple entries. The operations in the group ring have an interpretation as list operations. Ring addition reflects taking the union of lists, multiplication with an element of $z \in \boldsymbol{Z}$ reflects taking the union of z identical copies of a list. Multiplication of ring elements has a not so obvious meaning, however, this operation is very useful as well. It is just what we have to do if we want to find the coefficients and the exponents for the matrix product of two polynomials in the matrix P.

Clearly, the opposite element of a ring element $\lambda = \sum_{i \in Z_n} \lambda_i \, \underline{i}$ is the element $\sum_{i \in \boldsymbol{Z}_n} (-\lambda_i) \, \underline{i}$. We denote it by $-\lambda$. Note also, that $\underline{0}$ is the neutral element with respect to the group ring multiplication $*$, as can be easily seen from the definition of this operation.

8.8. EXAMPLE: In order to become acquainted with the operations in the group ring $\boldsymbol{Z}(\boldsymbol{Z}_n)$ and with the notation used here the reader should perform the following exercise. We still assume $n = 6$. Let

$$\sigma = 2\,\underline{0} + 3\,\underline{1} + \underline{2} + 3\,\underline{4}, \quad \tau = \underline{1} + 2\,\underline{2} - 3\,\underline{5},$$

then

$$\begin{aligned}
2\sigma &= 4\,\underline{0} + 6\,\underline{1} + 2\,\underline{2} + 6\,\underline{4} \\
\sigma \circ \tau &= 3\,\underline{1} + 2\,\underline{2} \\
\sigma + \tau &= 2\,\underline{0} + 4\,\underline{1} + 3\,\underline{2} + 3\,\underline{4} - 3\,\underline{5} \\
\sigma * \tau &= 2\,\underline{1} + 4\,\underline{2} - 6\,\underline{5} + 3\,\underline{2} + 6\,\underline{3} - 9\,\underline{0} + \underline{3} \\
&\quad +2\,\underline{4} - 3\,\underline{1} + 3\,\underline{5} + 6\,\underline{0} - 9\,\underline{3} \\
&= -3\,\underline{0} - \underline{1} + 7\,\underline{2} - 2\,\underline{3} + 2\,\underline{4} - 3\,\underline{5}.
\end{aligned}$$

Let $X = \{1,2,3\}$, $Y = \{1,4,5\}$. Then

$$\underline{X} * \underline{Y} = \underline{1,2,3} * \underline{1,4,5} = 2\,\underline{0,1,2} + \underline{3,4,5}.$$

In order to find $\underline{X} * \underline{Y}$ we have to calculate all sums $x \oplus y$, $x \in X, y \in Y$, and to list them. For X and Y as in the last calculation above this list is $2,5,0,3,0,1,4,1,2$. Then we look at the different entries of this list and note how often they appear. Since 0, 1 and 2 appear 2 times each we get the term $2\,\underline{0,1,2}$. The remaining entries appear just once each. This is expressed by the term $\underline{3,4,5}$.

8.9. Proposition. *The centralizer ring $\mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$ is isomorphic to the group ring $\boldsymbol{Z}(\boldsymbol{Z}_n)$. For $A = \sum_{i \in \boldsymbol{Z}_n} \lambda_i P_i \in \mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$ define*

$$\phi(A) = \sum_{i \in Z_n} \lambda_i i.$$

Then ϕ is an isomorphism from $\mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$ onto $\boldsymbol{Z}(\boldsymbol{Z}_n)$.

Proof. Being an isomorphism means that ϕ is bijective and that for $A, B \in \mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$ and $\rho \in \boldsymbol{Z}$ we have

$$\phi(A+B) = \phi(A)+\phi(B),\ \phi(AB) = \phi(A)*\phi(B),\ \phi(\rho A) = \rho\phi(A), \phi(A \circ B) = \phi(A) \circ \phi(B).$$

These properties of ϕ follow directly from the definitions of the ring operations in $\mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$ and in $\boldsymbol{Z}(\boldsymbol{Z}_n)$. ◇

Once more, note that for $A = \sum_{i \in I} \lambda_i P_i,\ B = \sum_{i \in J} \mu_i P_i$ we get

$$\phi(A \circ B) = \sum_{i \in I \cap J} (\lambda_i \mu_i)\, i.$$

Therefore, as already mentioned in subsection 8.4, the operation $\circ$ in $\boldsymbol{Z}(\boldsymbol{Z}_n)$ which corresponds to the S-H-multiplication in $\mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$ is

$$(\sum_{i \in I} \lambda_i i) \circ (\sum_{i \in J} \mu_i i) = \sum_{i \in I \cap J} (\lambda_i \cdot \mu_i) i.$$

In particular, for $X \subseteq \boldsymbol{Z}_n$ and $Y \subseteq \boldsymbol{Z}_n$

$$\underline{X} \circ \underline{Y} = \underline{X \cap Y}.$$

8.10. Let Γ be a circulant graph with adjacency matrix A. We want to find $<< A >>$. Proposition 8.9 tells us that this cellular ring will be isomorphic to some subring $\mathcal{S}$ of $\boldsymbol{Z}(\boldsymbol{Z}_n)$. $\mathcal{S}$ must reflect all properties of $<< A >>$, in particular, it must be closed with respect to the operation $\circ$ in $\boldsymbol{Z}(\boldsymbol{Z}_n)$. This requirements lead us to the following definition.

A subring $\mathcal{S}$ of a group ring $\boldsymbol{Z}(\boldsymbol{Z}_n)$ is called *Schur ring* or briefly *S-ring* over $\boldsymbol{Z}_n$ if

- (S1) $\mathcal{S}$ is closed with respect to addition and to multiplication with elements from $\boldsymbol{Z}$ (these are the conditions for $\mathcal{S}$ being a so-called $\boldsymbol{Z}$-module);

- (S2) There are simple quantities $\underline{T}_0, \underline{T}_1, \ldots, \underline{T}_d$ in $\mathcal{S}$ such that every element $\sigma \in \mathcal{S}$ has a unique representation

$$\sigma = \sum_{i=1}^{d} \sigma_i \, \underline{T}_i$$

(in which case this set of simple quantities is called a *basis* of $\mathcal{S}$);

- (S3) $\underline{T}_0 = \underline{0}$, $\sum_{i=1}^{d} \underline{T}_i = \underline{\boldsymbol{Z}}_n$;

- (S4) For each $i \in \{1, 2, \ldots, d\}$ there is a $j \in \{1, 2, \ldots, d\}$ such that $\underline{T}_j = \underline{-T}_i$ $(= \underline{\{\, n - x \; : x \in T_i \,\}})$;

By definition of a subring, $\mathcal{S}$ satisfies also

- (S0) For $i, j \in \{0, 1, \ldots, d\}$ there exist non-negative integers ρ_{ij}^k such that

$$\underline{T}_i * \underline{T}_j = \sum_{k=0}^{d} \rho_{ij}^k \underline{T}_k.$$

Indeed, for a subset $\mathcal{S}$ of $\boldsymbol{Z}(\boldsymbol{Z}_n)$ satisfying (S0) is equivalent to being closed with respect to the operation $*$. Hence, a subring $\mathcal{S}$ must satisfy this condition. It means that, if we write down a list of all possible sums $x \oplus y$ with $x \in \underline{T}_i$ and $y \in \underline{T}_j$, then for every k each element of $\underline{T}_k$ appears in this list with the same multiplicity ρ_{ij}^k.

The basis $\underline{T}_0, \underline{T}_1, \ldots, \underline{T}_d$ is called a *standard basis* of $\mathcal{S}$, the sets T_i are called *basic sets.* To relate an S-ring to its basic sets we shall write

$$\mathcal{S} = <\underline{T}_0, \underline{T}_1, \ldots, \underline{T}_d> .$$

The circulant graphs $\Gamma_i = \Gamma(T_i)$, $0 \le i \le d$, are called *basic circulant graphs* of $\mathcal{S}$.

$\boldsymbol{Z}(\boldsymbol{Z}_n)$ itself and $<\underline{0}, \underline{\boldsymbol{Z}_n - \{0\}}>$ are S-rings over $\boldsymbol{Z}_n$. Both of them are *trivial* S-rings. Clearly, we are mostly interested in non-trivial S-rings.

By definition, the automorphism group of an S-ring $\mathcal{S} = <\underline{T}_0, \underline{T}_1, \ldots, \underline{T}_d>$ is the intersection of the automorphism groups of the basic circulant graphs of $\mathcal{S}$, i.e.

$$Aut(\mathcal{S}) = \bigcap_{i=0}^{d} Aut(\Gamma_i).$$

8.11. Cellular subrings of the centralizer ring $\mathcal{V} = \mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$ and S-rings over $\boldsymbol{Z}_n$ are equivalent notions, as we are going to demonstrate in this paragraph.

Let $\mathcal{W} = <B_0, B_1, \ldots, B_d>$ be a cellular subring of $\mathcal{V} = \mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$. Assume

$$B_i = \sum_{l \in T_i} P^l, \; T_i \subset \boldsymbol{Z}_n, \; 0 \le i \le n-1$$

where the sets T_i form a partition of $\boldsymbol{Z}_n$. Consider the set

$$\mathcal{M} = \{\sum_{i=0}^{d} \lambda_i \underline{T}_i \; : \; \lambda_i \in \boldsymbol{Z} \quad \text{for} \quad 0 \leq i \leq d\}.$$

Since $\mathcal{W}$ is closed with respect to multiplication, for each pair i, j there are integers ρ_{ij}^k, $0 \leq k \leq d$, such that

$$B_i B_j = \sum_{k=0}^{d} \rho_{ij}^k B_k = \sum_{k=0}^{d} \rho_{ij}^k \sum_{l \in T_k} P^l.$$

On the other hand

$$B_i B_j = \left(\sum_{r \in T_i} P^r \right) \left(\sum_{s \in T_j} P^s \right) = \sum_{r \in T_i} \sum_{s \in T_j} P^r P^s = \sum_{r \in T_i} \sum_{s \in T_j} P^{r \oplus s}.$$

Hence,

$$\sum_{r \in T_i} \sum_{s \in T_j} P^{r \oplus s} = \sum_{k=0}^{d} \rho_{ij}^k \sum_{l \in T_k} P^l.$$

Now compare the entries in the first row of the matrices on both sides of this equality. The matrix $P^{r \oplus s}$ has a single entry equal to 1 at the position $t = r \oplus s$ in its first row. This entry appears on the left side as often as t appears in $\underline{T}_i * \underline{T}_j$. On the other hand, the first row of the matrix $\sum_{l \in T_k} P^l$ has entry 1 in exactly those positions which appear in the formal sum for the simple quantity $\underline{T}_k$. Hence from the equality above it follows that

$$\sum_{r \in T_i} \sum_{s \in T_j} r \oplus s = \sum_{k=0}^{d} \rho_{ij}^k \underline{T}_k$$

or

$$\underline{T}_i * \underline{T}_j = \sum_{k=0}^{d} \rho_{ij}^k \underline{T}_k.$$

Hence, $\mathcal{M}$ fulfills (S0). In a similar way, starting with (CA1) - (CA3), we find that $\mathcal{M}$ satisfies also (S1) - (S4). This shows that $\mathcal{M}$ is an S-ring over $\boldsymbol{Z}$, i.e.

$$\mathcal{M} = < \underline{T}_0, \underline{T}_1, \ldots, \underline{T}_d > .$$

Going back the way we just went, we can associate to each S-ring over $\boldsymbol{Z}_n$ a cellular subring of $\mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$. Hence, there exists a 1-to-1 correspondence between the set of all S-rings over $\boldsymbol{Z}_n$ and the set of all cellular subrings of $\mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$. Thus, and this is very important, we may replace all operations in $\mathcal{V}(\boldsymbol{Z}_n, \boldsymbol{Z}_n)$ by less cumbersome operations in $\boldsymbol{Z}(\boldsymbol{Z}_n)$.

8.12 Let us reformulate cellular expressibility (see 7.6) in terms of S-rings over $\boldsymbol{Z}_n$.

For circulant graphs $\Gamma_1 = \Gamma(X_1)$ and $\Gamma_2 = \Gamma(X_2)$ we have $\Gamma_1 \models \Gamma_2$ iff $\underline{X}_2$ belongs to the $S-$ring $<< \underline{X}_1 >>$ generated by $\underline{X}_1$ ($<< \underline{X}_1 >>$ is the smallest S-ring containing $\underline{X}_1$).

If this happens then $Aut(\Gamma_1) \leq Aut(\Gamma_2)$. We shall also use the notation $\underline{X}_1 \models \underline{X}_2$ in this case. In the next two paragraphs we mention two simple but important situations which will be met later again.

8.13. Lemma. *Let $X \subseteq \boldsymbol{Z}_n$. If $\underline{X} \models \underline{1}$ then $Aut(\Gamma(X)) = \boldsymbol{Z}_n$.*

Proof. Let $\mathcal{V} = \boldsymbol{Z}(\boldsymbol{Z}_n)$. $\underline{X} \models \underline{1}$ means $\underline{1} \in << \underline{X} >>$. However, $<< \underline{1} >> = \mathcal{V}$, hence $\mathcal{V} \subseteq << \underline{X} >>$. Since $\mathcal{V}$ is the largest S-ring over $\boldsymbol{Z}_n$, this implies $<< \underline{X} >> = \mathcal{V}$. Furthermore, $Aut(\Gamma(\boldsymbol{Z}_n, X)) = Aut(<<\underline{X}>>) = Aut(\mathcal{V}) = \boldsymbol{Z}_n$. $\diamond$

8.14. Let $X \subseteq \boldsymbol{Z}_n$. If $X = -X$, i.e. if $i \in X$ implies $-i = n - i \in X$, then $\Gamma(X)$ is an undirected graph. Remember that (i, j) is an edge of Γ iff $j - i \in X$. Hence, if both (i, j) and (j, i) are edges and if $x = j - i$, then $i - j = -x \in X$.

Lemma. *Let $X \subseteq \boldsymbol{Z}_n$, $X = -X$ and $\Gamma = \Gamma(X)$. If $\underline{X} \models \underline{1, n-1}$ then $Aut(\Gamma) = D_n$, the dihedral group, which is transitive and has order $2n$ and degree n.*

Proof. Recall that $\mathcal{D}_n$ includes the "rotations" $i \mapsto i \oplus h$ ($h \in \boldsymbol{Z}_n$ fixed) and the "reflections" $k \ominus i \leftrightarrow k \oplus i$ (again $k \in \boldsymbol{Z}_n$ fixed), and if n is even, $k \ominus i \leftrightarrow k \oplus 1 \oplus i$ (see also 4.32).

Start with the undirected circulant graph $C_n = \Gamma(\{1, n-1\})$ which is a closed polygon with vertices $0, 1, \ldots, n-1$. C_n is certainly invariant with respect to D_n, in fact $D_n = Aut(C_n)$.

Now, let $X_k = \{k, n-k\}$, $0 \leq k < \frac{n}{2}$. By definition of $<< \underline{X_1} >>$ we have $\underline{0}$, $\underline{X}_1 \in << \underline{X_1} >>$. It follows $\underline{X}_1 + \underline{X}_1 \in << \underline{X_1} >>$. However, for arbitrary $k < \frac{n}{2} - 1$ we have $\underline{X}_k * \underline{X}_1 = \underline{X}_{k+1} + \underline{X}_{k-1}$ or $\underline{X}_{k+1} = \underline{X}_k * \underline{X}_1 - \underline{X}_{k-1}$. Therefore, if $\underline{X}_0, \underline{X}_1, \ldots, \underline{X}_k \in << \underline{X_1} >>$ then $\underline{X}_{k+1} \in << \underline{X_1} >>$. From these arguments it follows $\underline{X}_k \in << \underline{X_1} >>$ for every $k < \frac{n}{2}$. A little more reflection shows that this is true also for $k = \frac{n}{2}$.

Now let us consider the graph $\Gamma(X)$. By assumption, $X = -X$, hence X is a union of some appropriate X_k, or equivalently, $\underline{X}$ is a (ring) sum of some appropriate $\underline{X}_k$. This implies $X \in << \underline{X}_1 >> = << \underline{1, n-1} >>$. Thus $\underline{1, n-1} \models X$ and therefore, since by assumption also $X \models \underline{1, n-1}$ is true, we get

$$Aut(\Gamma) = Aut(<< X >>) = Aut(<< \underline{1, n-1} >>) = Aut(C_n) = D_n.$$

$\diamond$

8.15. Example. Assume $n = 11$ and let $\Gamma = \Gamma(\{1, 2, 3, 4\})$. Find $Aut(\Gamma)$.
In $\boldsymbol{Z}(\boldsymbol{Z}_{11})$ we find

$$\underline{1, 2, 3, 4} * \underline{1, 2, 3, 4} = \underline{2, 8} + 2\,\underline{3, 7} + 3\,\underline{4, 6} + 4\,\underline{5}.$$

Application of Schur-Wielandt's principle gives

$$\underline{1, 2, 3, 4} \models \underline{2, 8},\ \underline{3, 7},\ \underline{4, 6},\ \underline{5}.$$

Furthermore,

$$\underline{1,2,3,4} \circ \underline{2,8} = \underline{2}, \quad \underline{1,2,3,4} \circ \underline{3,7} = \underline{3},$$
$$\underline{1,2,3,4} \circ \underline{4,6} = \underline{4}, \quad \underline{1,2,3,4} - (\underline{2} + \underline{3} + \underline{4}) = \underline{1}.$$

This proves $\underline{1,2,3,4} \models \underline{1}$. Therefore, due to Lemma 8.13, we have $Aut(\Gamma) = \boldsymbol{Z}_{11}$.

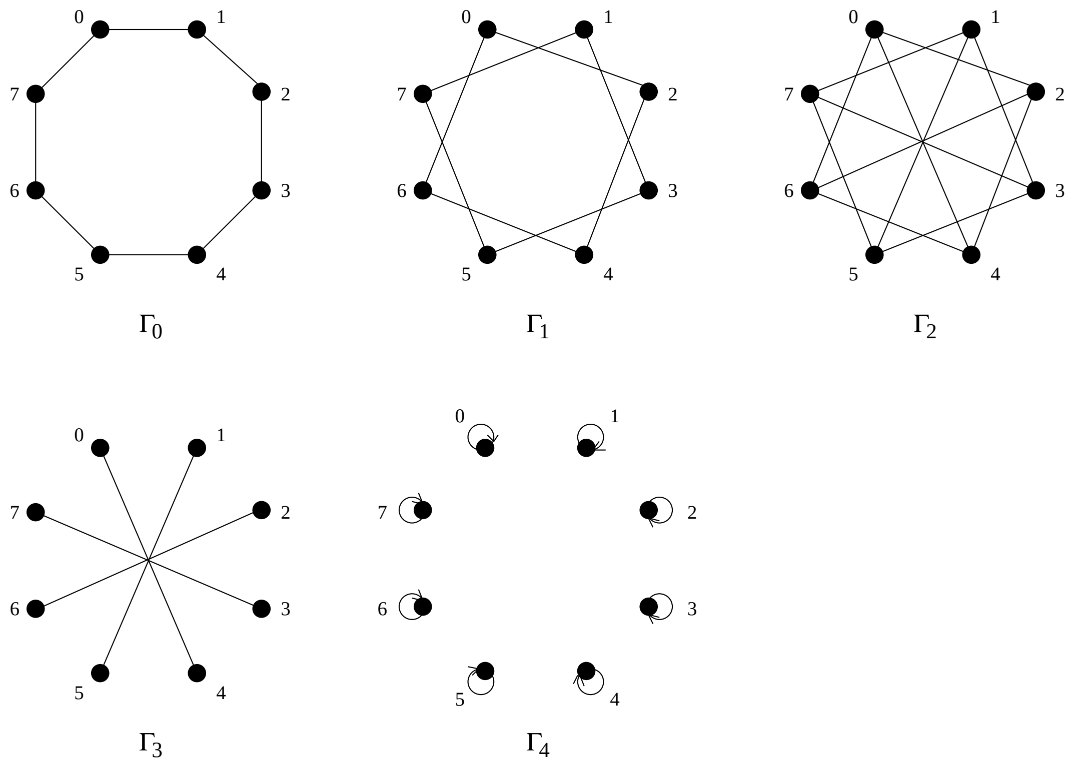


Figure 8.4.

8.16. Example. Describe the automorphism groups of all undirected 8-vertex circulant graphs.

We start with the S-ring $\mathcal{S}_0 = <\underline{0}, \underline{1,7}, \underline{2,6}, \underline{3,5}, \underline{4}>$. Next we list all S-rings over $\boldsymbol{Z}_8$ which are subrings of $\mathcal{S}_0$:

$$\begin{aligned}
\mathcal{S}_1 &= <\underline{0}, \underline{1,3,5,7}, \underline{2,6}, \underline{4}>, \\
\mathcal{S}_2 &= <\underline{0}, \underline{1,3,5,7}, \underline{2,4,6}> \\
\mathcal{S}_3 &= <\underline{0}, \underline{1,2,3,5,6,7}, \underline{4}> \\
\mathcal{S}_4 &= <\underline{0}, \underline{1,2,3,4,5,6,7}> .
\end{aligned}$$

Analysing this list we get

$$\mathcal{S}_0 = <<\underline{1,7}>>, \ \mathcal{S}_1 = <<\underline{2,6}>>, \ \mathcal{S}_2 = <<\underline{2,4,6}>>, \ \mathcal{S}_3 = <<\underline{4}>>, \ \mathcal{S}_4 = <<\underline{0}>> .$$

Hence, for $i \in \{0,1,2,3,4\}$ we have $Aut(\mathcal{S}_i) = Aut(\Gamma_i)$, where $\Gamma_0 = \Gamma(\{1,7\})$, $\Gamma_1 = \Gamma(\{2,6\})$, $\Gamma_2 = \Gamma(\{2,4,6\})$, $\Gamma_3 = \Gamma(\{4\})$, $\Gamma_4 = \Gamma(\{0\})$, see Figure 8.4.

Finally, we establish a complete list of the automorphism groups of these graphs:

$$\begin{aligned}
G_0 &= Aut(\Gamma_0) = D_8,\ |G_0| = 16,\\
G_1 &= Aut(\Gamma_1) = S_2 \wr D_4,\ |G_1| = 128,\\
G_2 &= Aut(\Gamma_2) = S_2 \wr S_4,\ |G_2| = 1152,\\
G_3 &= Aut(\Gamma_3) = S_4 \wr S_2,\ |G_3| = 384,\\
G_4 &= Aut(\Gamma_4) = S_8,\ |G_4| = 40320.
\end{aligned}$$

If $\Gamma = \Gamma(X)$ is any undirected circulant graph then first compute $<<\underline{X}>>$, next find i such that $<<\underline{X}>> = \mathcal{S}_i$ and finally get $Aut(\Gamma) = Aut(\Gamma_i)$. For example, $<<\underline{1,4,7}>> = \mathcal{S}_0$, hence $Aut(\Gamma(\{1,4,7\}) = D_8$.

8.17. S-rings over cyclic groups were introduced by the German algebraist I. Schur in his classical paper [Sch33]. S-rings can be considered in more general context over arbitrary groups. This extension was developed by disciples and followers of Schur, see [Wie64], [Koc66], [PosK79], [Sco64], [Tam70]. At the beginning, S-rings were used only for purely group-theoretical goals. Investigation of circulant graphs by means of S-rings started in [PosK79], [KliP81].

9 Automorphism groups of certain chemical graphs

9.1. In this section we shall demonstrate on a few examples how the techniques developed in the previous sections can be applied in order to find the automorphism groups of chemical graphs of different kinds. We shall restrict ourself to so-called *vertex transitive* graphs, i.e. to graphs with automorphism groups which act transitively on the vertex set of the graphs.

In each of our examples we consider an infinite series of graphs, the first members of the series being discussed in the chemical literature. In a first step we take an arbitrary graph Γ of the considered series and set up a certain "evident" subgroup H of $G = Aut(\Gamma)$. In the next step we then examine the conjecture : Is it true that $G = H$? Using rather simple computations in S-rings related to the considered series of graphs we prove that for most of the graphs in the series this conjecture is true. It may happen however, that we find also exceptional graphs for which the conjecture is not true. These graphs we have to investigate more carefully, thereby eventually finding additional automorphisms for them. In this way we finally describe their complete automorphism group.

9.2. Consider the graph representing the structural formula of a hydrocarbon. This graph contains a subgraph which consists of all carbon atoms of the molecule and of the bonds between them. In organic chemistry, this subgraph is called the *skeleton* of the hydrocarbon. A similar substructure appears in all heteroatomic organic compounds. For example, consider the structural formula Γ of the cyclopropane molecule which is depicted in Figure 9.1a. Its skeleton $\tilde{\Gamma}$ is shown in Figure 9.1b.

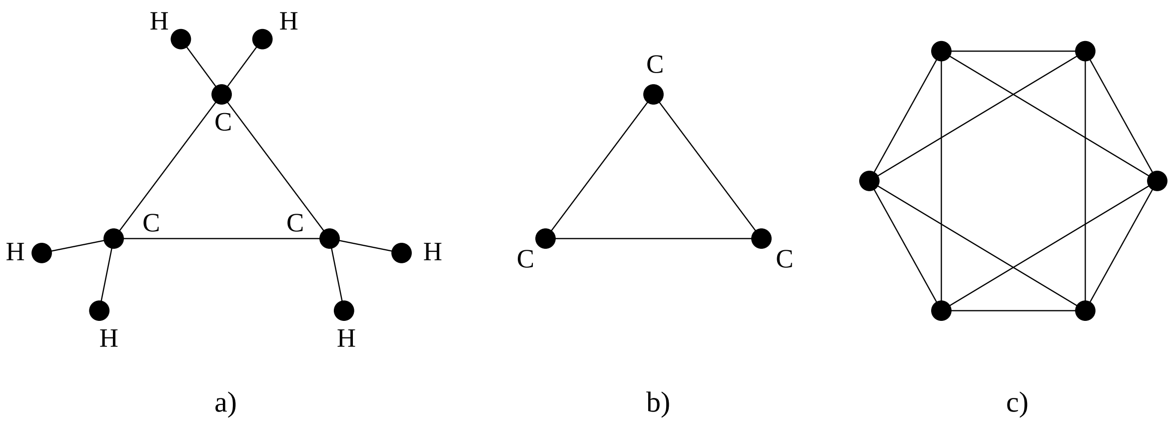


Figure 9.1.

The automorphism group of Γ is intransitive (since no hydrogen atom can change place with a carbon atom). Each automorphism of Γ can be thought of as two processes: First perform an arbitrary permutation of the carbon atoms (this is an automorphism of $\tilde{\Gamma}$), after this, permute the two hydrogen atoms, independently at each carbon atom. Hence, $G = Aut(\Gamma)$ is isomorphic to the wreath product $S_3 \wr S_2$ which is of order $3!\, 2^3 = 48$. The automorphism group $\tilde{G}$ of $\tilde{\Gamma}$ equals S_3. Hence, here the automorphism group of the skeleton serves as the "active" factor (outer group) in the wreath product. At this point, for a mathematician, the problem of finding the automorphism group of Γ is solved.

However, chemists usually do not use the notion of the wreath product for the description of automorphism groups of chemical graphs. Perhaps this is the reason why A. T. Balaban in [Bal78] introduced an artificial graph (which has no chemical meaning) in order to discuss the group G in question. This graph (we denote it by B_3) is shown in Figure 9.1c. There is no problem to find $Aut(B_3)$. Since $Aut(B_3) = Aut(\bar{B}_3)$ and since $\bar{B}_3$ (the graph complementary to B_3) is a disjoint union of three isolated edges (each edge representing a copy of the 2-vertex complete graph K_2), we have again $Aut(\bar{B}_3) = S_3 \wr S_2$.

9.3. In fact, Balaban investigated the automorphism groups of the structural formulas for all members of the homological series of cycloalkanes C_nH_{2n}. The graph Γ in the previous subsection represents the first member of this series, two other members will be considered below.

In [Bal78] an infinite series of graphs B_n was defined. For $n \in \boldsymbol{N}$, $n \geq 3$, B_n is a regular $2n$-vertex graph of valency 4. Actually, it is the circulant graph $\Gamma(\boldsymbol{Z}_{2n}, \{1, n-1, n+1, 2n-1\})$. This observation makes evident that the automorphism group G_n of the Balaban graph B_n contains the subgroup D_{2n} (the dihedral group of order $4n$ and degree $2n$). The edge set of B_n is a union of two 2-orbits of the group D_{2n} which correspond to the simple quantities $\underline{1, 2n-1}$ and $\underline{n-1, n+1}$ of $\boldsymbol{Z}(\boldsymbol{Z}_{2n})$.

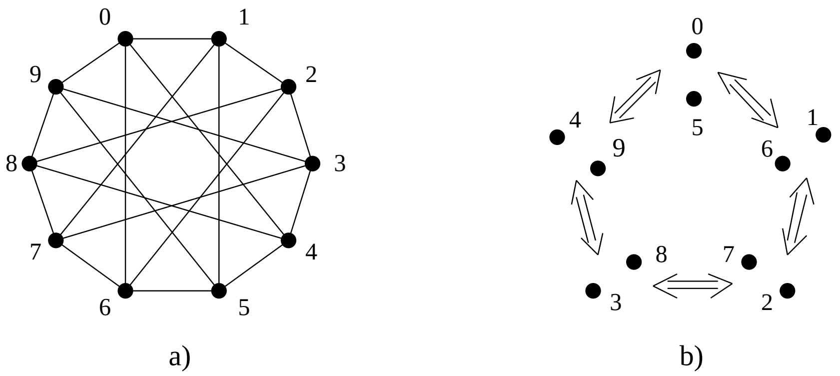


Figure 9.2.

9.4. Proposition. *Let $n \geq 3$ and $G_n = Aut(B_n)$. Then*

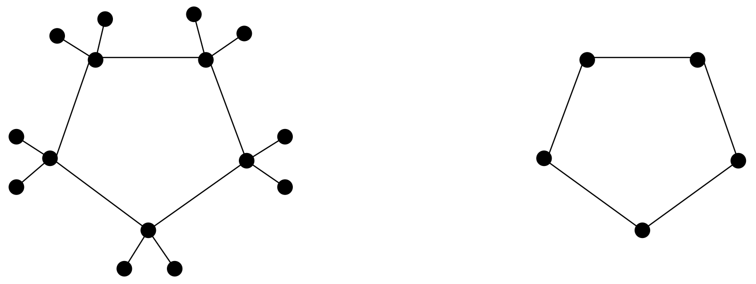
$$G_n = \begin{cases} D_n \wr S_2 & \text{if} \quad n \neq 4 \\ S_2 \wr S_4 & \text{if} \quad n = 4. \end{cases}$$

Proof. Let us start with the case $n = 4$. Again, we use $Aut(B_n) = Aut(\bar{B}_n)$. $\bar{B}_4$ is the disjoint union of two copies of the complete 4-vertex graph K_4. This shows that $Aut(\bar{B}_4) = S_2 \wr S_4$.

Now assume $n \neq 4$. Let us start with the graph B_5 which is depicted in Figure 9.2.a. Figure 9.2.b shows the same graph represented by a different diagram. Here each double arrow $\Longleftrightarrow$ denotes four edges between two pairs of vertices. For example, the double arrow between $\{0,5\}$ and $\{1,6\}$ denotes the edge set $\{\{0,1\}, \{0,6\}, \{1,5\}, \{5,6\}\}$. Figure 9.2.b makes evident that $G_5 \geq D_5 \wr S_2$.

In the same manner the inclusion $G_n \geq D_n \wr S_2$ is justified for each $n \geq 3, n \neq 4$.

In order to prove the inverse inclusion let us consider $X = \{1, n-1, n+1, 2n-1\}$. For $n \geq 5$ we get $\underline{X} * \underline{X} = 4\,\underline{0} + 4\,\underline{n} + 2\,\underline{2, n-2, n+2, 2n-2}$. Using Schur-Wielandt's principle, we find $\underline{X} \models \underline{n}$. Hence, for $n \geq 5$, each automorphism of B_n preserves the graph $\Gamma(\boldsymbol{Z}_{2n}, \{n\})$, or in other words, preserves the "supervertices $\{\{i, i+n\} : 0 \leq i \leq n-1\}$ of the diagram analogous to the diagram in Figure 9.2b. Changing "supervertices" to ordinary vertices and "superedges" (= double arrows) to simple edges in these diagrams we get an n-gon whose automorphism group is D_n. Let K be the subgroup of G_n which leaves each "supervertex" of B_n invariant. Then $|G_n| = |K| \cdot |D_n|$. The subgroup K consists of 2^n permutations which independently transpose or do not transpose the two vertices in each supervertex. Hence $|G_n| = 2^n \cdot 2n$. Taking into account that $|D_n \wr S_2| = 2^n \cdot 2n$, too, for $n \geq 5$, we get $G_n = D_n \wr S_2$. The case $n = 3$ was considered in 9.2. $\diamond$



a) b)

Figure 9.3

9.5. REMARKS. 1. The cyclopentane molecule C_5H_{10} and its skeleton are depicted in Figure 9.3.a and 9.3.b. Labelling of atoms is omitted. Graph B_5 in Figure 9.2.a,b serves as an artificial graph which has to describe the action of the automorphism group of the structural formula on the set of hydrogen atoms.

2. For $n = 4$, we have $\underline{X} * \underline{X} = 4\,\underline{0, 2, 4, 6}$, hence, $\underline{X} \models \underline{4}$ is not true. For this reason the automorphism group of B_4 is strictly larger than $D_4 \wr S_2$.

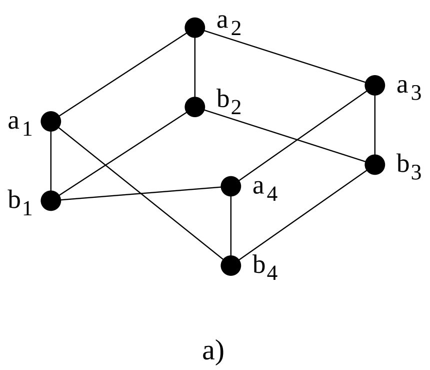
3. In [Bal78] Proposition 9.4 was claimed without proof and without exception for $n = 4$. Balaban when discovering this interesting rule did not recognize the existence of an exception for $n = 4$. In fact, the exception for cyclobutane ($n = 4$) is an artefact originating from the use of the Balaban graphs B_n. It is avoided when the usual constitutional formula and the notion of the generalized wreath product (in the sense of [ZefTK85]) are

used.

4. A rigorous formulation of Proposition 9.4 first appeared (without proof) in [ZefTK85] with reference to private communication to M.H. Klin. It was also announced in [KliKZ90].

5. The proof for Proposition 9.4 can be considered as an example for the usefulness of S-ring techniques. The wreath product and its generalizations, see e.g. [KerL77], [Bal84], [ZefTK85], are rather useful tools in the investigation of the symmetry of chemical graphs.

6. A rigorous proof of the claim $|G_n| = |K| \cdot |D_n|$ involves the notion of homomorphisms of groups. (In fact, D_n is the image of a homomorphism from G_n where $K = (\boldsymbol{Z}_2)^n$ is its kernel.)



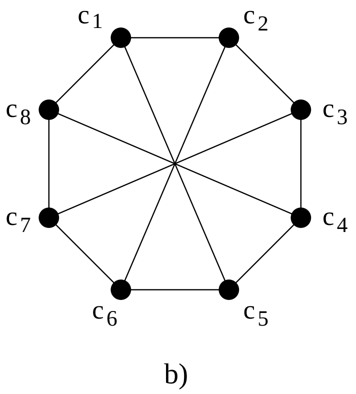


Figure 9.4

9.6. The graph of Figure 9.4.a is known as the *four-rung-Möbius-ladder*. This graph is nonplanar. It describes the structural formula of a representative of a new class of chemical compounds which were synthesized by D.M. Walba and his collaborators, see [WalRH82] and the references given in [WalSH88].

In fact, the synthesis of the first organic Möbius ladders was an important event in the development of modern theoretical stereochemistry, see e.g. [Wal87].

Because of some interesting chemical implications we would like to know the full automorphism group $Aut(M_4)$ of the graph M_4 in Figure 9.4.a. Again, as in the case of Balaban graphs, it is convenient to consider another isomorphic representation of M_4. The graph M_4' in Figure 9.4b is isomorphic to M_4, an isomorphism is given by the mapping

$$\begin{pmatrix} a_1 & a_2 & a_3 & a_4 & b_1 & b_2 & b_3 & b_4 \\ c_1 & c_2 & c_3 & c_4 & c_5 & c_6 & c_7 & c_8 \end{pmatrix}.$$

M_4' is evidently a circulant graph. Replace each label c_i by the new label $i-1$ in order to recognize M_4' as $\Gamma_4 = \Gamma(\boldsymbol{Z}_8, \{1,4,7\})$. Γ_4 is undirected, hence $Aut(\Gamma_4) \geq D_8$. We want to know the whole group $Aut(\Gamma_4)$. It turns out that the answer can be obtained within the framework of a more general discussion.

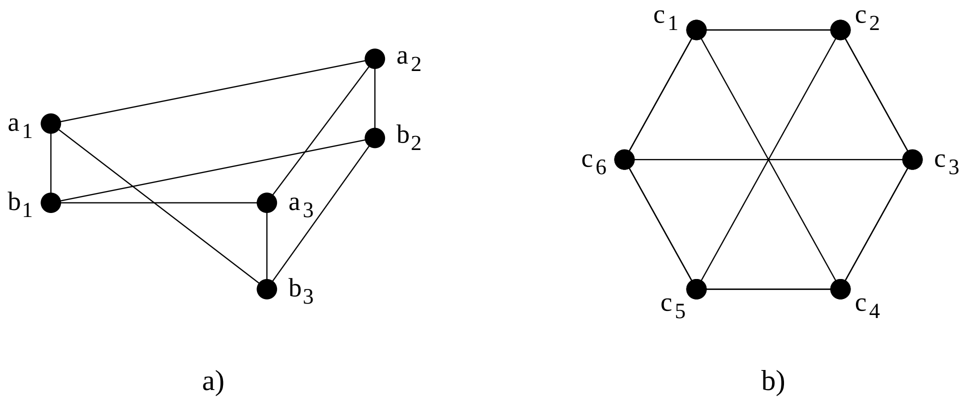


Figure 9.5.

9.7. Following [GuyH67], we define a Möbius ladder with n rungs to be a graph $M_n = (V, E)$ with $V = \{a_1, \ldots, a_n, b_1, \ldots, b_n\}$, $E = \{\{a_1, a_2\}, \{a_2, a_3\}, \ldots, \{a_{n-1}, a_n\}, \{a_n, b_1\}, \{b_1, b_2\}, \ldots, \{b_{n-1}, b_n\}, \{b_n, a_1\}, \{a_1, b_1\}, \{a_2, b_2\}, \ldots, \{a_n, b_n\}\}$. The graph M_n has $2n$ vertices, each vertex has valency 3. M_4 was considered above, M_3 is depicted in Figure 9.5.

Now, let us compare M_n with the graph $M'_n = (V', E')$ where $V' = \{c_1, c_2, \ldots, c_n, c_{n+1}, \ldots, c_{2n}\}$ and $\{c_i, c_j\} \in E'$ if and only if

$$(j - i)(mod\, 2n) \in \{1, n, 2n - 1\}.$$

Here, $(j - i)(mod\, 2n)$ means $j - i$ if $j - i \geq 0$, and means $2n + j - i$ if $j - i < 0$.

9.8. Lemma.
(a) The graphs M_n and M'_n are isomorphic;
(b) M'_n is isomorphic to the circulant graph $\Gamma_n = \Gamma(\boldsymbol{Z}_{2n}, \{1, n, 2n - 1\})$.

Proof. (a) Define

$$\phi(a_i) = c_i,\ \phi(b_i) = c_{i+n},\ 1 \leq i \leq n.$$

It is easily checked that $\phi : V \longrightarrow V'$ is an isomorphism of M_n and M'_n.
(b) Define the mapping $\psi : V' \longrightarrow \boldsymbol{Z}_{2n}$ by

$$\psi(c_i) = \begin{cases} i & \text{if} \quad 1 \leq i \leq 2n - 1 \\ 0 & \text{if} \quad i = 2n, \end{cases}$$

ψ is an isomorphism of M'_n and Γ_n. ◇

9.9. Consider the dihedral group D_{2n} as a group acting on $\boldsymbol{Z}_{2n}$. We know that the centralizer ring $V = V(D_{2n}, \boldsymbol{Z}_{2n})$ is isomorphic to the S-ring

$$\mathcal{S} = <\underline{0}, \underline{1, 2n-1}, \underline{2, 2n-2}, \ldots, \underline{n-1, n+1}, \underline{n}>$$

over $\boldsymbol{Z}_{2n}$. Hence, each of the three isomorphic graphs M_n, M_n' and Γ_n can be associated with the simple quantity $\underline{X} = \underline{1, n, 2n-1}$.

9.10. *Proposition. For* $n \geq 3$

$$Aut(\Gamma_n) = \begin{cases} D_{2n} & \text{if} \quad n > 3, \\ S_2 \wr S_3 & \text{if} \quad n = 3. \end{cases}$$

Proof. Assume $n = 3$. The complement graph $\bar{\Gamma}_3$ is the disjoint union of two triangles. Hence, $Aut(\Gamma_3) = Aut(\bar{\Gamma}_3) = S_2 \wr S_3$. The order of $S_2 \wr S_3$ is $2 \cdot (3!)^2 = 72$.
Now assume $n > 3$. Because of $X = -X$ we can use Lemma 8.14. Due to this Lemma, to prove the present proposition it suffices to prove that $\underline{X} \models \underline{1, 2n-1}$. We have

$$\underline{X} * \underline{X} = 3\,\underline{0} + \underline{2, 2n-2} + 2\,\underline{n-1, n+1}.$$

According to Schur-Wielandt's principle we get $\underline{X} \models \underline{2, 2n-2}$. Now

$$\underline{X} * \underline{2, 2n-2} = \underline{1, 2n-1} + \underline{3, 2n-3} + \underline{n-2, n+2}$$

and

$$(\underline{X} * \underline{2, 2n-2}) \circ \underline{X} = \underline{1, 2n-1}.$$

Hence, $\underline{1, 2n-1} \in << \underline{X} >>$ which is the same as $\underline{X} \models \underline{1, 2n-1}$. ◇

9.11. Corollary. *For $n > 3$ the group $Aut(M_n)$ has one orbit on the set of vertices of M_n (a 1-orbit) and two orbits on the set of edges of this graph (one 2-orbit consits of the rungs and the second 2-orbit consists of the uprights of M_n). $Aut(M_3)$ has one orbit for vertices and one orbit for edges.*

9.12. Comments and Remarks.
1. For $n = 3$ we have $\underline{X} * \underline{2, 4} = 2\,\underline{X}$, hence we cannot prove $\underline{X} \models \underline{1, 5}$. For this reason $Aut(\Gamma_3)$ is larger than D_6.

2. Proposition 9.10 was first proved using *ad hoc* arguments in [Sim86], see also [WalSH88]. The present idea of a proof was previously announced in [KliKZ90] and [FarKM94].

3. In [Sim86] and [Fla89] finding $Aut(M_n)$ was considered as introduction to the more intriguing problem of determining the topological symmetries of a given molecule (here the attribute "topological" is correct, compare with the remark in section 3.2). The topological symmetry of a molecule is closely related to its topological equivalences and topological chirality. It reveals deep and natural links between mathematics and theoretical stereochemistry.

In fact, in [Sim86] each automorphism of M_n was examined with respect to the possibility of the representation of it by a suitable isotopy of the 3-sphere S^3. By inspection of all such isotopies it was possible to prove that for $n \geq 4$ there is no isotopy of S^3 which maps

M_n onto its mirror image, i.e. M_n is *chiral* for $n \geq 4$.

4. Corollary 9.11 states an important fact. Let us consider a real Möbius ladder molecule including in each edge of M_n, $n \geq 4$, the same number of additional carbon atoms. Then, as discussed in [WalSH88], the additional carbon atoms will be distinguishable, e.g. by means of ^{13}C NMR. Here one signal will correspond to the atoms situated in the rungs while a second signal is expected for the atoms situated on the uprights of the Möbius ladder. Note that according to Corollary 9.11 in the case $n \geq 4$ the rungs form a 2-orbit of $Aut(M_n)$ different from the 2-orbit of the uprights.
(An excellent survey [Bal95b] provides the reader an opportunity to get acquaintance with various other interrelations between combinatorics and spectroscopy.)

5. The graph M_3 is isomorphic to the famous Kuratowski graph $K_{3,3}$, one of the two graphs which are responsible for the non-planarity of a graph, see [Har69].

9.13. Let us return to example 5.27 where we considered the pentagonal prism P_5. We have found that $Aut(P_5) \geq G$, where G is a certain group of order 20. Chemists denote this group by D_{5h}. In mathematical notation we have $G \cong D_5 \times S_2$, $D_5 = \langle g_1, g_2 \rangle$, $S_2 = \langle g_3 \rangle$. Let us find the whole group $Aut(P_5)$.

Let A be the adjacency matrix of P_5 and A_i the adjacency matrices of the graphs $\Gamma_i = (\Omega, \Phi_i)$, $0 \leq i \leq 5$. It is evident that $\{\Gamma_1, \Gamma_3\} \models P_5$. We shall demonstrate that also $P_5 \models \{\Gamma_1, \Gamma_3\}$ is true. Check that

$$A^2 = 3A_0 + A_2 + 2A_4.$$

Hence, due to Schur-Wielandt's principle, A_0, A_2, A_4 are cellularly expressible by A. Now we obtain

$$AA_4 = 2A_3 + A_1 + A_5.$$

Again using Schur-Wielandt's principle we get $A_3 \in \langle\langle A \rangle\rangle$. Finally, $A_1 = A - A_3$. Thus, $P_5 \models \{\Gamma_1, \Gamma_3\}$.

Now, since $\langle\langle A \rangle\rangle = \langle\langle A_1, A_3 \rangle\rangle$, we have $Aut(P_5) = Aut(\Gamma_1) \cap Aut(\Gamma_3)$. $Aut(P_5)$ is transitive, because its subgroup G is transitive. Let $g \in Aut(P_5)$, $g \neq e$, such that $1^g = 1$. This implies $6^g = 6$ (because Γ_3 is regular with valency 1). In turn from this it easily follows that $g = g_2$, hence the stabilizer of vertex 1 in $Aut(P_5)$ has order 2. Finally, we get $|Aut(P_5)| = 10 \cdot 2 = 20$, and therefore $Aut(P_5) = G$.

9.14. For $n \geq 3$ let P_n be the graph which is made up by the skeleton of an n-gonal prism. This graph has vertex set $\Omega = \{1, 2, \ldots, 2n\}$ and edge set

$$E = E_1 \cup E_2 \cup E_3$$

where

$$E_1 = \{\{1,2\},\ \{2,3\},\ \ldots,\{n-1,n\},\ \{1,n\}\,\}$$

$$E_2 = \{\{n+1, n+2\}, \ldots, \{2n-1, 2n\}, \{n+1, 2n\}\}$$

$$E_3 = \{\{1, n+1\}, \{2, n+2\}, \ldots, \{n, 2n\}\}.$$

9.15. Proposition. For $n \geq 3$

$$Aut(P_n) = \begin{cases} D_n \times S_2 & \text{if} \quad n \neq 4, \\ S_4 \times S_2 & \text{if} \quad n = 4. \end{cases}$$

The group $D_n \times S_2$, as an abstract group, is isomorphic to D_{nh}. Its order is $4n$. $S_4 \times S_2$ has order 48, see subsection 6.15.

The proof of the proposition for $n \neq 4$ can be given by a reasoning completely analogous to the one in the previous subsection.

10 Concluding Remarks

10.1. We conclude the paper with a brief historical review of the development of the ideas explained here. We shall call the reader's attention to the most important events, we do not attempt to deliver a complete picture. Additional details can be found in other surveys, see references below. Also some reminiscences related to personal experiences of the authors will be included.

10.2. Forerunners.
Certainly, the origin of coherent algebras is found in the classical paper [Sch33]. There Schur introduced a new notion which later by his students was called an S-ring. Schur used S-rings for the solution of an important group-theoretical problem posed by W. Burnside. During some decades this purely group-theoretical line was the only source of interest in S-rings.

The paper by Schur stimulated the development of an alternative approach using double coset classes. In [Man39] Schur's results were arrived at by this approach once more (this was one of the last papers by W.A. Manning, a classic of permutation group theory). In a series of papers, see for example [Fra41], [Fra48], J.S. Frame showed how the basis of a centralizer algebra of a prescribed permutation group (transitive or intransitive) can be constructed by means of double coset classes. In [Fra48] the reader can find as an example the adjacency matrix of a centralizer algebra of rank 17 for an intransitive permutation group of degree 18. The author's interest in the subject stems from the study of molecular structures. Frame mentions that

> "the potential energy of the molecule is approximated by a quadratic form whose matrix V must commute with all the matrices of the symmetry group of the molecule. Its characteristic roots are closely related to the molecular spectrum."

In fact, a common use of the commuting matrices is one of the important tools in the classical quantum theory, cf [Wig59].

10.3. Invention of association schemes.
The theory of association schemes was born in India, at the Statistical Laboratory at Calcutta (now the Indian Statistical Institute). This laboratory was involved in mathematical modelling in agricultural field experimentation. The theory of randomised and Latin square block designs created by R.A. Fisher and F. Yates (see e.g. [Fis35], [Yat37]) makes it possible to study arrangements of v varieties of treatments in b blocks of k different varieties each. In a classical balanced incomplete block design (BIBD) each variety occurs in the same number r of blocks, and also every pair of varieties occurs in the same number λ of blocks. BIBD's are ideal models for statistical experiments, nowadays they are used universally, including in chemistry (see [KagS83], [Kag88]). Unfortunately, BIBD's exist for rather specific sets of parameters (v, b, k, r, λ) only. This causes severe restrictions for their use. As an alternative, partially balanced incomplete block designs (PBIBD) were introduced by R.C. Bose and K.R. Nair in 1939 in [BosN39]. A PBIBD has also the above mentioned parameters v, b, k, r, however all pairs of different varieties

are classified into m classes, called *associates*, such that each pair from the i-th associate occurs together λ_i times, $1 \leq i \leq m$. Thus, the necessary conditions for the existence of PBIBD's are weaker than those for BIBD's. This fact creates more opportunities for their use.

The axioms for PBIBD's are divided into two parts, one part being responsible for the requirements of the associate classes. They define a class of combinatorial structures which are called *association schemes.* Although these axioms first appeared in [BosN39], the term itself was introduced by R.C. Bose and T. Shimamoto in [BosS52].

In fact, Bose and Nair have also suggested, and illustrated with illuminating examples, the most important methods for the construction of association schemes and PBIBD's, which are classified by them as:

- use of simple geometrical configurations,
- application of finite geometry
- methods of differences
- application of the duality principle between blocks and varieties.

A reader acquainted with modern mathematical ideas will certainly be surprised to find at the very origin of the theory of association schemes the main principles of almost all important methods for constructing these combinatorial objects. Naturally, the papers [BosN39] and [BosS52] have stimulated numerous publications, most of them devoted to the construction of new PBIBD's, in particular with $m = 2$ classes. Results of these activities were summarised in [BosCS54] and [Cla56].

The final step in the invention of association schemes was their "algebraisation." Graphs were considered which have treatments as vertices and pairs from the i-th associate class as arcs ($1 \leq i \leq m$). The adjacency matrices of these graphs generate a matrix algebra of order v and rank $m + 1$ which later became known as Bose–Mesner–algebra (BM–algebra) of an association scheme. This algebra turns out to be isomorphic (in the commutative case) to a smaller algebra of order $m + 1$ (the latter fact is outside our exposition, see for details [BanI84]). This algebraic reformulation was independently discovered by W.A. Thompson in 1954 in his doctoral thesis (see also [Tho58]), by R.C. Bose in 1955 and by D.M. Mesner in 1956. In 1959 the two latter authors have published the joint paper [BosM59], which now is considered as one of the classical sources of Algebraic Combinatorics. Bose and Mesner have developed the foundations of character theory of BM-algebras as a partial case of linear associative algebras. Let us add the remark that the term "association" originally referred to "associate" = "partner, colleague, companion" etc., but by no means to "associative" in its well–known mathematical meaning.

10.4. Centralizer algebras.

We have already mentioned that centralizer algebras of permutation groups were first used by I. Schur, W.A. Manning and J. S. Frame (in rather different terminology). Their investigations were continued, on a more general base, by H. Wielandt, a student of Schur. Wielandt's first publication on this subject [Wie36] was already mentioned by Manning in [Man39] as "remarkable for its brevity". A detailed introduction into the theory of centralizer algebras first appeared in Wielandt's well–known book [Wie64] (its preliminary rotaprint version was available earlier and is based on lectures delivered in 1954/55). This book is still one of the best sources for the theory of finite permutation groups.

We believe that Wielandt was not acquainted with the papers on association schemes. However, in his book he introduced (in terms of S-rings) a class of structures which can be interpreted as association schemes, but which cannot be described as sets of 2-orbits of a suitable permutation group. In terms of cellular algebras his examples can be interpreted as examples of such algebras which are not centralizer algebras. We call such algebras *non–Schurian* cellular algebras, because Schur believed that each S-ring implies a suitable centralizer ring (in fact, Schur himself dealt only with S-rings over cyclic groups, and for this particular case his conjecture seems to be true). Within the frames of association schemes theory first examples of non-Schurian BM-algebras were given by L.G. Chang, A.J. Hoffman, D.L. Mesner and S.S. Shrikhande in 1956-1960, see [Cha59], [Shr59], [Hof60], [Cha60] (the example of D.L. Mesner appeared in his unpublished thesis, 1956).

10.5. Rank 3 groups.
A group is called *simple* if it has no non-trivial invariant normal subgroups. The first examples of simple groups were given by E. Galois. The efforts of several mathematicians during more than one century resulted in the discovery of certain infinite families of simple groups and of five sporadic simple groups. New examples of sporadic simple groups were discovered rather recently, in 1965-1975. One of these examples by D.G. Higman and Ch. Sims, a simple group of order 44 352 000, was found as a rank 3 subgroup of index 2 in the automorphism group of a 100-vertex graph [HigS68]. Thus, this group was found by construction of a new rank 3 coherent algebra. In the same manner a few other examples of new simple groups were found.

The success of Higman and Sims was based on their previous experience in the investigation of permutation groups. In particular, Higman's papers [Hig64] and [Hig67] had a profound impact on the development of modern permutation group theory.

10.6. Strongly regular graphs.
Let $W =< A_0, A_1, A_2 >$ be a symmetric cellular algebra of rank 3. The matrices A_1, A_2 are the adjacency matrices of two graphs Γ_1, Γ_2 which in this case are called *strongly regular graphs*. They are complementary to each other. In other words, an undirected n-vertex graph Γ is called strongly regular if and only if its adjacency matrix $A = A(\Gamma)$ satisfies

$$A^2 = kI_n + \lambda A + \mu\bar{A}$$

for suitable parameters k, λ and μ ($\bar{A}$ is the adjacency matrix of the complementary graph $\bar{\Gamma}$.)

A strongly regular graph is called a *rank* 3 graph if $Aut(\Gamma)$ is a rank 3 permutation group. Strongly regular graphs which are not rank 3 graphs serve as examples for non-Schurian coherent algebras. In fact, the above mentioned examples by Mesner–Shrikhande and Chang–Hoffman are strongly regular graphs with 16 and 28 vertices, respectively.

The term "strongly regular graph" was introduced by R.C. Bose in [Bos63]. In this paper Bose considered links between strongly regular graphs and partial geometries (special classes of finite incidence structures).

The detection of simple groups by investigating automorphism groups of graphs initiated an explosive growth of interest in rank 3-graphs and in strongly regular graphs as their natural generalization. Several different new techniques related to strongly regular graphs were introduced by J.J. Seidel and his collaborators, see e.g. [Sei67], [Sei68], [GoeS70], [BerLS73], [Sei76], [CamGS78]. For getting deeper acquaintance with the subject we recommend the survey papers [Sei69], [HesH71], [Hub75], [BroL84].

10.7. Coherent configurations.
At the end of the 60's the independently developed theories of association schemes and centralizer algebras had reached so high a level that it became inevitable to merge them as well as to create generalizations of association schemes which could serve as "combinatorial approximations" to the set of 2-orbits of arbitrary permutation groups (transitive or intransitive). This mission was fullfilled by D.G. Higman.

In his paper [Hig70] Higman introduced the notion of coherent configurations on a set X as a pair $(X, \mathcal{P})$ where $\mathcal{P}$ is a partition of $X \times X$ which satisfies certain axioms. To each configuration there is a corresponding matrix algebra, in fact this correspondence is a bijection. At the beginning, Higman termed this algebra the centralizer ring of a coherent configuration, later, in [Hig75], an adjacency algebra (ring), and finally, in [Hig87], a *coherent algebra*. In our paper the last term is adopted, together with the term cellular algebra with unit. In Higman's terminology, cells (= BM-algebras of association schemes) correspond to homogeneous coherent configurations. In other words, homogeneous coherent configurations are equivalent to association schemes. Higman published several papers, in particular lecture notes of two courses [Hig72] and [Hig77], which helped a rather wide part of the mathematical community to adopt and to use the notion of coherent configuration. The origin of Higman's interest in coherent configurations is to be found in group theory, representation theory of semisimple algebras and finite geometries. However, in his more recent publications he also expressed interest in computational problems and in particular in WL-stabilization (see e.g. [Hig90]).

10.8. Cellular algebras.
One of the origins for the Weisfeiler–Leman approach to cellular algebras were papers on centralizer algebras of permutation groups (in particular [Hig67]). Surprisingly, at the beginning, Weisfeiler and Leman did not realize the existence of non-Schurian cellular algebras. We stress that [WeiL68] was published before Higman's axiomatization, so that at the beginning the notions of cellular and coherent algebras were developed quite inde-

pendently.

In [Lem70] all cellular algebras of order $n \leq 7$ and all cells of order $n \leq 9$, as well as their automorphism groups (in terms of generators) were described, all necessary computations were made by hand. The first example of a (non-Schurian) strongly regular graph having intransitive automorphism group ($n = 26$) was found using a computer and reported in [AdeWLF69]. Impressive results of a method for constructive enumeration of strongly regular graphs were represented in [ArlLR75]. The method was based on a computer program for canonization of graphs which was elaborated by I.A. Faradžev and his coworkers (see [ArlZUF74]). These and other results of the booming Moscow school were summarised in [Wei76].

Unfortunately, for some while all the absurdities and humiliations of Soviet life were a serious obstacle for the development of this promising scientific research group. As a result, Leman gave up the subject and started a career as an expert in system programming. Weisfeiler emigrated from the USSR. He never returned to Algebraic Combinatorics.

10.9. Kalužnin's school.
L. A. Kalužnin (1914-1990) was born in Moscow but spent more than 30 years in Germany and in France. He was one of the last students of Schur. In 1955 Kalužnin returned to the USSR and founded the Department of Algebra and Mathematical Logic at Kiev State University.

As already mentioned a few times, the late 60's were a surprisingly fruitful and creative time for interdisciplinary influences and interrelations. Just at this time Kalužnin organised a seminar on "Galois theory of relational algebras." Starting from the old paper by M. Krasner [Kra38], the participants of this seminar became successful in the uniform treatment of Post algebras, transformation semigroups and permutation groups, having a given set of invariant relations, see [BodKKR69] (and [PosK79] for further developments). As part of this activity great attention was paid to the description of maximal subgroups of symmetric and alternating groups as automorphism groups of suitable relations (preferably graphs). The first papers in this area are mentioned in Section 1. A detailed survey of the results in permutation group theory achieved by Kalužnin's school can be found in [FarKM94], [Ust94] (see also [FarIK90], [SusKLPUV98]).

In [KalK72] and in subsequent papers each permutation group (G, Ω) was considered as the automorphism group of a suitable set $\mathcal{K}$ of k-ary relations with suitable $k \in \boldsymbol{N}$. This set $\mathcal{K}$ is closed with respect to certain set-theoretical operations and is called a *Krasner algebra* (see [KalK72], [KliPR88] for details). If (G, Ω) is 2-closed then the corresponding Krasner algebra $\mathcal{K}$ is generated by binary relations, however, in general this is not the case. It turns out that the occurence of a non-Schurian cellular ring can be explained in terms of Krasner algebras. Roughly speaking, such rings are closed with respect to the usual binary operations on matrices, but they are not closed with respect to suitable multiary operations (which can be associated with so–called high stabilization). Simple versions of such k-ary operations ($k > 2$) were discussed by Wielandt in [Wie64], [Wie69], and in papers related to strongly regular graphs, see e.g. [HesH71], [BroIK89]. A detailed exposition of all these questions and of their interrelations with results from [Fur87] and [CaiFI92] will be the subject of the third paper of our series.

At the beginning, the members of Kalužnin's school were not well-acquainted with the Weisfeiler-Leman approach. They used the term V-ring, which in [Kli78] was first changed to cellular subring of a centralizer ring. At the same time (in 1978) I. A. Faradžev and several of his students together with M. Klin began a long and fruitful collaboration of the Kiev and Moscow schools.

10.10. Association schemes: an explosion of interest.
The paper [Del73] (P. Delsartes's doctoral thesis) is considered as one of the best monographs on association scheme theory. This important link between combinatorics and algebraic coding theory has widely enlarged the use of association schemes.

Almost at the same time N. Biggs (see [Big74], [Big76]) posed certain problems related to the notion of *distance regular graphs* (a generalization of strongly regular graphs). The existence of a distance regular graph of diameter d implies the existence of a so–called p-polynomial association scheme with d classes.

The notion of 2-orbits (proposed by Wielandt in [Wie69] and adopted in [KalK72]) as well as the equivalent notion of an *orbital graph* of a transitive permutation group (introduced by Sims) became rather popular due to such papers as e.g. [Sim67-68], [Qui71], [Kna73], [Cam74], [Neu77].

Within a few years the interest in association schemes grew explosively. The results of the initial period of their development have been summarised by E. Bannai and T. Ito in [BanI84]. Their bibliography includes 404 items (not including the results of the Soviet school which were absolutely unknown to mathematicians in the West till the appearance of the paper [Iva83] by A. A. Ivanov). An additional 163 references will be found in two supplements to the Russian translation of [BanI84] which was published in 1987. Nowadays association scheme theory is a well-developed part of algebraic combinatorics. A significant amount of its results are reflected in [BroCN89], [God93], [Zie96].

10.11. Algebraic combinatorics.
The reader without mathematical training certainly has become confused by the stream of new notions and references to be encountered in the previous subsections. In fact, this is only a minor part of the available information. We believe that this part will help to realize the existence of a new wide area of mathematics and of its links with numerous subjects in mathematical chemistry. To our knowledge the name "algebraic combinatorics" for this area was used first in [BanI84]. During recent years it has almost completely replaced the older term "algebraic graph theory".

In fact, algebraic combinatorics (as it is used, say by Math. Reviews), covers a wider part of mathematics, including such subjects as formal power series, incidence algebras of partially ordered sets, Möbius inversion, symmetric functions, Burnside rings etc. The books [Sta86], [Ker91] are recommended as excellent guides to these areas. However, here we conceive the term "algebraic combinatorics" in a restricted sense, i.e. in the sense of Bannai and Ito.

Besides the above mentioned monographs association schemes have been discussed also with respect to various other topics. In particular, chapters on association scheme theory can be found in [Dem68], [CveDS80], [MacS78], [LinW92].

Computational aspects of coherent algebras are discussed in [Fri89], [Pon93], [FarKM94].

10.12. Due to the elementary level of our presentation it is not possible to submit here a detailed and deep survey of algebraic combinatorics. Much interesting information will be found in [BanI84]. Additional historical details are mentioned in [Kli85], [KliF86], [FarIK90] and [FarKM94]. In a few lines only we add some examples of questions which are not touched otherwise in this section.

Finite geometries play a significant role for the establishment of association scheme theory. We prove this by two illustrations:
(A) F. Levi, one of the founders of modern discrete geometry (see [Lev29]), after his emigration from Germany worked at the University in Calcutta. His six public lectures [Lev42] delivered at this university helped researchers in design of experiments to become acquainted with literature which was not available in India.
(B) For many mathematicians the book [Dem68] by P. Dembowski was the first source for getting acquainted with association schemes. In particular, it was cited by Higman in [Hig70].

Modern spectral and structural theory of BM-algebras (it is out of our scope here) in its main features has been developed many years ago by O. Tamaschke for the case of S-rings, see e.g. [Tam64], [Tam68], [Tam70]. A more general approach is developed in [Zie96].

Classification of finite simple groups has been achieved as a result of 25 years collective effort of hundreds of mathematicians (the size of all papers related to the complete proof is of about 10000 pages), see [Gor82]. This classification implied numerous important consequences in modern mathematics, in particular, in algebraic combinatorics.

Certain other questions which are closely related to the main line of the present paper will be briefly discussed in the final subsections.

10.13. Double cosets.
Let G be a group and F, K two of its subgroups. For each $g \in G$ define

$$FgK = \{\, fgk \mid f \in F,\ k \in K \,\}.$$

This set is called a *double coset* of G with respect to F, K. If $F = K$ then FgF is called a double coset with respect to F.

The set of all different double cosets of G with respect to F forms a partition of G. Moreover, simple quantities coresponding to double cosets generate a Schur subring of the group ring $Z(G)$ which is denoted by $H(G, F)$. This ring is called a *Hecke ring* (*Hecke algebra*, if the coefficients are taken from $\mathbb{C}$).

Let (G, Ω) be a transitive permutation group, $a \in \Omega$, $F = G_a$ the stabilizer of the point a. It turns out that the centralizer algebra $V(G, \Omega)$ is isomorphic as an abstract algebra (anti-isomorphic in the non-commutative case) to the Hecke algebra $H(G, F)$, for details see [BanI84], [FarKM94].

In more sophisticated terms analogous anti-isomorphisms can be established for centralizer algebras of intransitive permutation groups.

Thus, in principle, all information related to centralizer rings of permutation groups (including structure constants and generalised adjacency matrices) can be described in terms of double cosets.

Double cosets themselves are well-known in group theory from the time of A.L. Cauchy onwards, see [Cau846]. The notion of Hecke algebras goes back to E. Hecke [Hec37]. Hecke algebras in evident form but in different terminology were used first by Manning and Frame (see above). To our knowledge Frame was the first to use double cosets in chemistry.

Nowadays, double coset techniques give examples of deep and wide applications of group-theoretical methods in chemistry. Below we mention only a small selection from the related bibliography: [HasR73], [BroHM74], [HasRKS79], [Fra79], [BroGW83], [RucK83], [Has85], [Bro86] (the titles give also a list of several important lines of applications).

The papers [KliTZ91], [KliZ91], [LloJ98] and [Bro94] are examples for the discussion of reaction graphs of degenerate rearrangements of chemical compounds in terms of 2-orbits and double cosets, respectively. The use of 2-orbits for this purpose goes back to [JonL83].

Enumeration (constructive and analytical) of chemical isomers is perhaps the best illustration of the fitness of double cosets in theoretical chemistry, see [KerL98] for a clear description of all necessary concepts.

We intend to discuss the interrelations between relational and double coset approaches for the application of centralizer algebras in combinatorics in a future paper. Roughly speaking, the enumeration of strongly regular graphs and the enumeration of all graphs illustrate the advantages of the first and the second approach, respectively. The automorphism group of a graph is usually determined in terms of the first approach. Double cosets seem to be very effective in constructive enumeration of substituted isomers (which appear via coloring of ligands of a prescribed molecular graph).

10.14. The main subject of this paper can now be reformulated as the problem of classifying pairs of vertices in a given graph Γ. The set of 2-orbits of $Aut(\Gamma)$ gives a solution to this problem. This set can be found by efficient algorithms which are presented in [FarK91], [FarKM94]. However, there is no proof of a polynomial time bound for the complexity of these algorithms.

The notion of a cellular ring (coherent configuration) serves as a rather good combinatorial approximation of the centralizer ring (the set of 2-orbits). The minimal cellular ring $\mathcal{W}(A)$ which includes the adjacency matrix $\mathrm{A} = A(\Gamma)$ can certainly be constructed in polynomial time.

As was mentioned in Section 3, during more than 20 years chemists were not aware of the Weisfeiler-Leman approach or its analogs. The first attempts of classification of pairs of vertices in chemical graphs were done in terms of distances between vertices [CarSV85]. The notion of 2-orbits stayed unused by chemists. However, G. Rücker and Ch. Rücker elaborated for use in the chemical world an algorithm for the classification of pairs of vertices which is based on the computation of powers of the adjacency matrix. This work is similar to the Weisfeiler–Leman approach.

Starting in September 1990, the four authors of the present paper tried to create a common understanding of the subject. We believe that the level of explanation of our paper can be considered as a convenient compromise between different standards traditionally adopted in mathematics and chemistry. Moreover, we hope that this paper will serve as a background for future interdisciplinary investigations and applications.

We have tried in this paper to overcome not only the evident difficulties of communication between mathematicians and chemists but also to smoothen the differences between the terminology used in cellular algebras and the theory of coherent configurations (as was already mentioned, during almost 20 years the Soviet school worked in complete isolation). In our opinion, the relational terminology of coherent configurations can be naturally combined with the matrix terminology of cellular algebras. Certain patterns of this combination can be observed in the previous sections.

10.15. Graph stabilization as it was suggested by Morgan [Mor65] is the common starting point of all origins of this paper (see e.g. [WeiL68], [Tin76], [HinT77], [RueR90b]). We were not able to explain this technique thoroughly within the framework of the present paper (Part I). However, it is the main subject of two subsequent papers of the series. Part II (which is written by L. Babel, M. Klin, I.V. Chuvaeva and D.V. Pasechnik) is devoted to detailed considerations of the Weisfeiler-Leman stabilization procedure, its theoretical complexity and its program implementation. In a more general context several different stabilization procedures are considered in Part III. In particular, we shall consider stabilization of depth k (deep stabilization in terms of [Wei76]). For $k = 2$ it coincides with the so–called total degree partition. An algebraic interpretation of the total degree partition in terms of doubly stochastic matrices was first achieved by G. Tinhofer in [Tin86] and [Tin91]. An information about the preliminary versions of the parts II, III is now available from the home page of G.Tinhofer.

WL-stabilization coincides with stabilization of depth 3. It was a long–standing question whether there exist cellular algebras which are stable with respect to stabilization of depth k, $k \geq 4$, but which are not centralizer algebras of suitable permutation groups. Finally, examples of such algebras for $k = 4$ and $k = 5$ have been given in [Iva87], [Iva89] and [BroIK89]. Examples for arbitary values of k have been given in [Fur87] and [CaiFI92], however, the presentation in the latter papers is very sophisticated and difficult to understand. We plan to give a revised and friendly interpretation of Fürer's examples in further parts of this series.

10.16. We hope that our series of papers will help to create new standards in mathematical chemistry and, first of all, will help to bridge the gap between the current achievements in algebraic combinatorics and the actual level of treatment of the graph isomorphism problem in mathematical chemistry.

There is one more point which deserves steady attention: the relationship between geometrical and combinatorial symmetry of molecular graphs. The legitimity of using the whole automorphism group in chemical informatics is, of course, beyond every question. However, for "internal" purposes chemists still prefer to give a convenient geometrical interpretation to each symmetry of a molecular graph. The first attempt of an extension of the traditional geometrical vision of symmetry was done by H. C. Longuet-Higgins in [Lon63]. Other attempts were done in [Hin79] and, in particular, in [Dre79]. A very detailed discussion of the symmetry properties of molecules can be found in [Ezr82] and [UgiDKM84]. Nevertheless, the use of "honest" combinatorial symmetry is still a very rare event in chemical papers. We hope to investigate this phenomenon in all its consequences. The final goal of this activity is to create a rigorous and clear mathematical description of what a chemist does when trying to identify or differentiate similar arrangements of atoms (in mathematical terms, the goal is to create suitable equivalence relations on the set of spatial arrangements of the atoms which describe a given molecule). The first attempt to do this, which can be found in [TraZ87], [KliTZ90], is not yet very well developed and can serve as a preliminary hint only. Moreover, graph-theoretical models are not sufficient for an adequate mathematical description of molecules. Impressive examples of the limitations of purely graph-theoretical ideas have been known to chemists since the early development of the structural approach to organic chemistry. For example, Crum Brown in [Cru864] was not able to explain (in the terms of constitutional formulae) the difference between maleic acid and fumaric acid, or between optically active and inactive malic acid, etc. Only the interplay between graph theory and discrete geometry will give sufficient mathematical background for a suitable description of all organic molecules. The elaboration of a convenient rigorous mathematical model for chemical stereoconfigurations is still one of the most challenging problems in mathematical chemistry.

10.17. This paper is a revised version of the technical report which was published in 1995 as a preprint TUM-M9510 of the Mathematical Institut, Technical University Munich. During the last few years a number of new important publications related to the subject of our series, appeared, for example [LaiCI97], [Fau98]. Unfortunately, we were not able to survey these publications in Part I.

Unless more convenient otherwise M. Klin should be regarded as the corresponding author.

11 Acknowledgements

M. Klin would like to express his deep gratitude to I. A. Faradžev, S. S. Tratch and N. S. Zefirov for a long-standing cooperation.

The initial outline of this paper was elaborated in July 1991 in Freiburg (Germany) in frames of a non-formal miniseminar on "Applications of permutation groups in chemistry". We are all obliged to O. H. Kegel for organizing this fruitful opportunity.

Other very helpful opportunities to test the presentation of some parts of the material have been arranged in spring 1995 while G. Tinhofer was visiting Ben-Gurion University of the Negev in Beer-Sheva (Israel), and during his subsequent visits there. The participation and extracurricular activity of A. Altshuler, J. Bernstein and his students at this university is sincerely appreciated.

In particular, we are highly indebted to E. K. Lloyd and S. S. Tratch who carefully read the preliminary version of this paper and made numerous substantial suggestions for its improvement. Their help is gratefully appreciated.

Finally, we thank L. Joergensen for an essential help in the checking the proofs of the final version of this paper.

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