Hanno van Keulen

MAKING SENSE

Simulation-of-Research in Organic Chemistry Education

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Making Sense

Simulation-of-Research in Organic Chemistry Education

Verstandig Maken
Simulatie-van-Onderzoek in Organisch-Chemisch Onderwijs
(met een samenvatting in het Nederlands)

Proefschrift

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Contents

1 Introduction

What is organic synthesis? Whatever it is, its accomplishments are all around us. The ink of my printer, the sweetener in my coffee, the aspirin I just took for a headache–all are products of organic chemical synthesis. You cannot simply find these substances out on the street, nor in nature. They were made, invented, by human beings, to serve human purposes. Organic synthesis thus is *making*. But people are not born with the capacity for making substances. Nor are they born with reasons for making new substances. This is something that has to be learned. Competence in organic synthesis is not acquired easily. Organic synthesis is not a part of the daily life of ordinary people. The products of organic synthesis may be everywhere, the processes are hidden inside laboratories and factories. Sometimes, organic synthesis is compared with cooking. There are similarities: in both processes a product is created that meets certain requirements. But organic synthesis is not entirely like cooking; indeed, in some respects it is entirely different.

This study investigates organic synthesis from an educational point of view. More specifically, I investigate the relations between teaching and learning organic synthesis in a university chemistry curriculum. I especially focus on the laboratory course for first year chemistry students at Utrecht University. "If one takes the view that laboratories are important places where knowledge is generated and validated in the experimental sciences, and if students are to gain an appreciation of these processes and to develop the abilities to contribute to them, then scientific inquiry could be regarded as the *raison d'être* of laboratory-based learning" (Boud, Dunn, & Hegarty-Hazel, 1986). I took this view. Consequently, I investigated laboratory-based instruction in organic synthesis to determine whether 'students gain an appreciation of' and 'develop the abilities to contribute to' scientific organic synthesis. My thesis is that chemistry students have to make *sense* of organic synthesis to be able contribute to it. Consequently, much attention is devoted to what exactly 'making sense' is in the context of organic synthesis.

In chapter 2, which is called 'The cookbook problem', I describe a preliminary investigation. I analyze the objectives and contents of the curriculum for first year university chemistry students at Utrecht University with respect to organic synthesis. From the title of this chapter it can be deduced that the results were not entirely positive. There is a problem, and this problem arises when organic synthesis is equated with cooking. Too much of instruction is based on recipes, which guide the student towards excellent chemical products, but which do not necessarily help them to understand the process. It is this understanding of the process that I am interested in, for I focus on students that are being educated to do chemical research. Therefore, the students do not only have to be able to achieve excellent results, they also need to understand the rationales of organic synthesis. I describe a detailed case study on the synthesis of aspirin. I conclude that, although the students are able to execute the prescriptions and obtain high yield and purity, they do not understand the rationale behind the prescription.
Of course, this cookbook problem is known to chemistry educators, and many solutions have already been proposed. I therefore analyze some of these proposals, to find that they are not entirely satisfactory. What I am looking for is a kind of instruction that prepares

students for doing research in such a way that there is an explicit relation between the teaching material and the learning results. I find that most solutions either still rely on prescriptions, or have only an implicit relation between teaching and learning.

In chapter 3, 'A hermeneutic framework', I therefore analyze science education from a more fundamental, philosophical point of view. My thesis is that many scientists apply an objectivist philosophy to education. They presume that science is about correct and objective descriptions of how things really are. This philosophical position suggests that science education can consist of the transfer of these descriptions, plus demonstrations of how to handle the equipment. As a result, science education consists of lecture courses in which the facts and theories are transferred, and laboratory courses in which these topics are illustrated and laboratory techniques are trained. I argue that this approach cannot be sufficient to prepare students for research. Scientists do not just describe 'how things really are'; they do this by taking a specific viewpoint. They have a question. So, I suggest to replace the objectivist approach to science education by an approach that takes viewpoints into account. I have found the foundations of such an approach in the hermeneutic philosophy of Hans-Georg Gadamer. Hermeneutics stresses the importance of viewpoints and context for giving meaning to knowledge. Hermeneutics holds that understanding is part of a process, a hermeneutic cycle of interpretation-understanding-application. The experience of an issue that is not understood leads to interpretation; this interpretation is explicated in language; and the resulting understanding is applied again to the issue at hand. This issue consequently acquires a different meaning. In chapter 3, I elaborate this hermeneutic framework for science education. My thesis is that students should understand, in the hermeneutic sense, in order to be able to do research.

Chapter 4 then applies this theoretical framework to develop a methodology that suits my research question. I argue that several conventional approaches to research in science education do not illuminate the process of understanding. I advance an interpretive methodology that is context-specific with regard to organic synthesis. The methodology, which is called the research cycle, suggests that I design new educational contexts. In these contexts, students experience chemical phenomena, interpret these, come to an understanding, and apply their understanding in a subsequent cycle. Something analogous should happen with the teacher: the teachers have experiences with students who are learning chemistry. They interpret, understand and apply in a similar fashion. Lastly, the researcher interprets the whole educational context, comes to an enhanced understanding of learning and teaching organic synthesis, and applies this to redesign the educational context.

Chapter 5, 'Interpretation', describes the first attempt at conducting educational research according to the hermeneutic research cycle. I designed an educational context, called Esters, in which students had to investigate processes of making esters. I describe this educational context in detail, including my intentions and expectations. I then interpret students' activities and this helps me to understand the possibilities and weaknesses of the design. I find that I can interpret students' understanding meaningfully in terms of three concepts: synthesis-planning, reaction-type, and structure-activity-relations. However, students' understanding of these concepts can only develop if the educational context allows them to explicate their own hypotheses and conduct their own experiments. This character of the educational context I unite within the concept of simulation of (organic-chemical) research.

In chapter 6, 'Understanding', I apply my understanding acquired through interpreting the first educational context by redesigning this context. I show that in this context students can achieve an understanding of the relations between the various stages in organic synthesis, especially between formation and purification. They understand the equilibrium reaction-type. And, they develop an understanding of the Lewis formalism to represent structure-activity-relations, especially with respect to localized charges in molecular formulae. In all these cases, 'understanding' implies the capacity for application in the context of organic synthesis, not just the capacity to give correct answers to test questions.

In chapter 7, 'Application', I give students the opportunity to apply their understanding of the three concepts in an expanded educational context, called Ethers. The creation of this educational context itself is an application of my own understanding of teaching and learning organic synthesis. In this context, students attempt to synthesize three unsymmetrical ethers. They apply their understanding of synthesis acquired through Esters, and discover new elements of synthesis-planning and a new reaction-type, the side-reaction. My attempt to expand their understanding of structure-activity-relations to include delocalized charges is not entirely successful. I trace this down to a problem in the educational context regarding simulation-of-research. The students' research-like questions and experiments focus on the product of synthesis, whereas they do not investigate questions from a theoretical viewpoint.

In the final chapter I discuss this latter problem to suggest lines for future research. I conclude that the hermeneutic approach can be applied with success to educational research in organic synthesis. I also engage in a discussion of my results concerning the teacher's cycle. In order to apply the hermeneutic approach to education as such, and implement the results of this study, it will be necessary to adopt a non-objectivist approach to teaching and to teacher education.

2 The cookbook problem

Organic synthesis is manipulation of matter, involving all kinds of activities and equipment usually associated with a laboratory. How do students learn this? How is it taught? What are the accepted ways of teaching organic synthesis? Do problems exist with teaching and learning, and if so, how are these tackled? How do I choose a framework to develop and answer specific research questions that are both interesting and resolvable? It seems sensible to start a study on these questions by exploring laboratory education. In this chapter, I therefore describe a preliminary investigation into organic chemistry laboratory courses.

Although the incorporation of laboratory work in chemistry education is not utterly undisputed since budget problems often urge educational institutions to look for cheaper alternatives, it is not very daring to state that most chemistry educators advocate the inclusion of laboratory work: "Practical work would be deemed by most chemists to be an essential ingredient of chemical education" (Johnstone & Wham, 1982).
In this quotation, the term 'practical work' is used instead of laboratory work. In the Dutch language, the term *practicum* is very common. To avoid confusion, I will use terms like these–and others, such as 'laboratory course'–throughout this study to refer to instruction in which students work in a laboratory with real substances.

2.1 The cookbook problem

Laboratory courses are not without problems. In this section I analyze a problem that has haunted chemistry laboratory courses for decades: the *cookbook problem*.
A common feature of almost all laboratory instruction is the *prescription*. Students have to follow written instructions that determine the practical work to a large extent. It is considered a problem is that they do not always seem to *understand* what they are doing, although they often carry out the instructions correctly. This cookbook problem can be seen as an undesired side-effect of laboratory instruction using prescriptions: "The absence of objectives makes it difficult for the student, who may read the experiment for the first time immediately prior to commencing the laboratory work, to realize what is going on. Yet because the procedure is so clearly detailed, the student is able to complete the exercise and achieve a result. It is not difficult to understand why, in the absence of clear reason for the activity, students see such exercises as cookbook or recipe work" ((Boud, et al., 1986) p. 37). And: "There is abundant evidence that even directly after completing a conventional practical exercise, many children cannot say what they did, why they did it, or what they found" (Hodson, 1990).
Especially the organic synthesis lab is criticized. Pickering, for example, writes: "Organic labs have degenerated into cooking. [...] A cook is concerned only with the creation of a product while an organic chemist wants the answer to a question" (Pickering, 1984).
Kandel nicely formulates the problem as: "The fault of many organic experiments seems to be that there are no questions asked and no thinking done, only instructions given to allow students to obtain products whose properties are matched to known values" (Kandel & Ikan, 1989). These observations are confirmed by many others (Cooley, 1991; Fife,

1968; Pickering, 1985; Potter & McGrath, 1989; Venkatachelam & Rudolph, 1974; Wade, 1979; Warren & Pickering, 1987).

The criticism in the literature on the cookbook problem focuses on the fact that most organic synthesis experiments are conducted with what is often called a *recipe*–a complete description of the laboratory actions that have to be carried out to obtain a fixed yield and purity. Students obtain correct chemical results but this does not necessarily result in understanding.

Teachers seldom seem to find fault with themselves. What they teach is sound and valid chemistry, in their own eyes. When nothing is wrong with instruction, the problem must lie with the student. Consequently, some teachers blame the students: they are lazy, lack motivation, are simply not intelligent enough, or something was wrong with their prior education (Wruck & Reinstein, 1989). Sometimes, this may even be true. However, students also criticize the cookbook lab. Roth writes: "The students indicated during interviews that they were quite aware of the difference between the open-inquiry and traditional laboratory exercises they conducted in their chemistry course. Most students did not like the cookbook approach of traditional laboratories because the purpose of most steps remained hidden from them" (Roth, 1994).

In any case, chemistry instructors are virtually powerless when it comes to influencing students innate capacities or prior knowledge. Hence, I think it is better to focus on the curriculum. Although this might appear as an innocent and obvious remark, it will have far-reaching consequences. *In my opinion, it is of little use to determine how students are learning in a curriculum that lacks internal validity.* Since I eventually had to draw this conclusion, I also had to develop a methodology that enabled me to do educational research on non-existing laboratory instruction. I will report on this development in the next two chapters.

Arguably, in many occasions understanding is not necessary. Indeed, the goal of a recipe–in cooking as well as in chemistry–is to get results; not to foster understanding. Not everybody needs to really understand chemistry. In many situations and professions it suffices to carry out instructions. But there is at least one category of students–future chemists–who should understand chemistry. Their education cannot be based on 'cookbooking' only. I focus on these students.

This study can be seen as an attempt to solve the cookbook problem. However, my aim is not just to develop an alternative set of experiments. I primarily try to develop a fundamental *understanding* of teaching and learning in organic synthesis, and to design an educational theory with which such alternatives can be created.

2.2 Process learning versus content learning

The content and organization of a curriculum depend on its objectives. Why do we teach students organic synthesis? Why must they conduct experiments? What do we want them to learn? In short: which are the objectives for education in organic synthesis? An important issue is whether the curriculum aims at preparing students for doing chemistry, or whether chemistry teaching is a means to attain other goals. The objectives of an organic synthesis course depend on the place organic chemistry has in the curriculum as a whole. I think it is appropriate to pay attention to some differences between the educational systems of various countries.

In the United States of America it is not uncommon for high school graduates to have taken only one year of chemistry. The first years of tertiary education aim at a broad and general education, in which all students take courses in various fields, including the natural sciences. Hence, large universities have freshman chemistry courses for thousands of students each year, whereas only some fifty-odd of these will eventually major in chemistry. Even less will go on to graduate school to do a PhD in chemistry. Both high school and the first years of college seem to emphasize what is indicated with *process-learning*: students should acquire *general cognitive skills* about such things as logical thinking, verbal and written communication, and problem solving; they should also develop positive attitudes towards science, culture, and society.

In The Netherlands, as in many European countries, education is oriented more towards what is indicated with *content-learning*. Students are supposed to go to an educational institution to master the *specific* content of subjects like foreign languages, history, and the sciences. A chemistry student in a Dutch university typically has had four years of secondary school chemistry, five years of physics, and six years of mathematics. Students choose their major field the moment they enter university. In the natural sciences, the curriculum is largely fixed and mandatory, and there is little opportunity nor obligation to take courses outside science. This difference is reflected in speech: American students 'take' courses, whereas Dutch students 'follow' courses. The Faculty of Chemistry at Utrecht University attracts on average one hundred students a year. Some sixty per cent of these will eventually graduate. No other students follow courses together with chemistry students since students from disciplines like biology and medicine have their own chemistry courses. Non-science majors do not take any science courses at all; they are supposed to have acquired sufficient understanding of the sciences in secondary school.

Given this difference, one would expect numerous and important differences between college chemistry in the U.S.A. and in The Netherlands. The needs of non-majors are quite different from the needs of those who plan to become professional chemists. The second group might expect to learn the basics of chemistry and be prepared for advanced courses. The first group might expect to get an impression of what chemistry is and how chemists get to know their facts. However, most American colleges do not provide different courses for majors and non-majors. With respect to chemistry, the differences between the two systems are quantitative rather that qualitative. Dutch freshmen start at a more advanced level, and they devote more time to chemistry. On the other hand, the lab facilities of Dutch secondary schools are not as good as those of American colleges, so these latter have the opportunity to teach the basics of chemistry with more emphasis on laboratory work. The chemistry itself does not seem to be essentially different. American textbooks and laboratory manuals cover the same material, use the same organizational principles, and describe the same experiments as their Dutch counterparts. Dutch universities often use American textbooks.

Although this suggests that chemistry education in both contexts is comparable with regard to content and structure, the objectives may nevertheless be different. In the U.S.A., the attainment of process skills is an important objective in its own right. In Europe, content comes first. Process skills are a by-product. As a consequence, chemistry education in Holland loses its validity if the chemistry in it is inaccurate, since the chief objective is chemistry learning. In the United States, regardless of the quality of the chemistry, the curriculum will be positively evaluated if students show enhanced general skills. Anyone who brushes through a few issues of the (American) Journal of Research in Science Teaching will be convinced that science teaching very often is investigated from this general-process-skills point of view.

I do not deny that, while learning chemistry, students can and should learn many valuable things of non-chemical nature. For example, chemistry often makes use of symbolic manipulations and calculations, so it can be expected that chemistry learning has as a by-effect enhanced competence in calculation skills. The same holds for logical thinking, propositional and proportional reasoning, and spatial thinking. However, I have two reasons not to commit research along this line. First, many chemical skills are very specific and do not transfer easily to other areas: "It is difficult to see, for example, in what sense the ability to use a pipette and burette successfully, in volumetric analysis, is transferable to a laboratory context in which an oscilloscope or microscope is to be employed or a dogfish to be dissected. It is even more difficult to see how such a skill can be transferred to a non-laboratory situation in everyday life" (Hodson, 1993). The reverse is also true: students who do well on general skills tests are not necessarily good chemists. Second, I do not see why chemistry should be chosen as a vehicle for enhancing non-chemical skills. It seems to me that the general skills mentioned can be fostered far better by subjects that have a more logical and less empirical structure.

In this study, therefore, I investigate chemistry education for future chemists from the content-specific point of view. Consequently, chemical validity is of crucial importance.

2.3 Objectives for teaching organic synthesis

If a curriculum should be valid from the viewpoint of chemistry, the objectives for education must be determined by what is necessary to achieve competence in doing research. The standards for this are determined by professional organic chemistry. The activities of professional organic chemists provide the ultimate justification for content and organization of education in organic chemistry, since we prepare students for jobs in these areas. For the sake of this study, I need a profile and not a detailed analysis, so my survey will be fairly general.

In general, chemistry students are prepared to understand science and to be able to do scientific research, both in a fundamental and in an applied context. In research, the simplest reason for conducting organic synthesis is that the product is directly useful for some purpose. Another reason is to find a substance with certain predetermined properties. Turner calls this the "examination of 'structure-activity' relationships" (Turner, 1976). A third reason to conduct synthesis is to confirm hypotheses regarding the structure of a substance through logically constructed synthetic routes. Finally, organic synthesis plays a part in the investigation of theoretical ideas on reaction mechanisms.

To prepare students for this, it should be known what it is when someone is able to carry out scientific research in the field of organic chemistry. I will restrict myself to those qualifications that are typical of organic chemistry and that can be learned. Thus, I will not pay explicit attention to many otherwise also important qualifications, such as, for example, creativity and responsibility.

I suggest that an adequate approach is to differentiate between *individual* aspects and *situated* aspects. Focusing on an individual chemist, one can see that he or she reads and writes scientific articles, uses various books, tables and graphs, and manipulates various sorts of glassware, apparatus, and substances. To be able to do these things the chemist has to have knowledge and understanding of facts, theories, models, substances, molecular formulae, reactions, mechanisms and principles; to have the skills to handle the equipment and to interpret data; and to be able to solve problems, that is, to formulate and answer research questions. These aspects can be called the *professional qualities.* Regardless of any instructional organization it is clear that objectives concerning the development of these professional qualities should be included.

A chemist is not an individual, working in solitude. The way a chemist conducts research is influenced largely by situated and cultural aspects. "The foundation of actions in local interactions with the environment is no longer an extraneous problem but the essential resource that makes knowledge possible and actions meaningful" (Hennessy, 1993). The activities derive their meaning from current research questions, which in turn are influenced by the paradigms of Western science in general and the specific research area in particular. What counts as an interesting question and an acceptable explanation in specific fields such as organic chemistry is decided by complicated processes of communication within a research community. Sociology of science has drawn attention to these processes (Fleck, 1979; Latour & Woolgar, 1986). An understanding of this *situated character* is indispensable to participate in the communicative processes, and thus to conduct research. So, any curriculum claiming to prepare future organic chemists should pay attention to these aspects too.

The professional qualities, so it seems, can be grouped into two categories: theory (or knowledge) and practice (or skills). This at least is suggested by the current educational practice to teach through lecture courses said to emphasize theory and through laboratory courses focusing on practical aspects. Although it may thus seem possible to distinguish between knowledge and skills, these cannot be isolated from each other without the risk of losing contact with the situated character of research. *In the profession, techniques as well as theories are used in a context determined by the research questions.* They always come together and give proper meaning to each other in each specific context. "A crucial element of learning science is knowing what knowledge is appropriate in particular circumstances, and being able to access and use it to meet particular needs and purposes" (Hodson, 1993). An example: distillation can be regarded as a technique for purifying liquids, and could be trained as such. However, what counts as 'pure' is determined by the needs of a specific situation. This situation therefore determines which specific distillation technique is most suitable.

Education should beware of the risk of treating the constituents of the profession separately while leaving the integration to the students. It is important to include objectives concerning the context in which to apply knowledge and skills. That context is scientific inquiry.

This point is advanced by several educational researchers. For example, Boud et al. write: "Unless at some stage students learn about the processes of scientific inquiry through being engaged in it, it is unlikely that they will be in a position to reach a full appreciation of the practice of science and be able to contribute to this enterprise themselves" (Boud, et al., 1986). This still leaves two questions open. One is: at which stage should student start with this 'being engaged in scientific inquiry'? Right from the start? If not, what do students learn in the preliminary stages and how do these look like? The other question is, what exactly is 'being engaged in'? Is research an all-or-nothing affair, which one can only learn by doing, or is it conceivable to 'learn about the processes of scientific inquiry' by being engaged in adequate educational situations not necessarily leading to new research results?

This general reflection has not yet made clear how to achieve the objectives. But it will suffice to serve as a background for a comparison with a real curriculum. In the next section, I investigate textbooks and laboratory manuals, and the official curricular documents of the Faculty of Chemistry at Utrecht University. I then investigate the actual educational situation at Utrecht University. I will also compare the results, to find out whether the three approaches lead to compatible views on objectives. After all, many differences are possible. Professional chemists can say things about educational goals that are not compatible with their own research, and they may disagree among each other. Textbook authors also may verbalize different opinions concerning objectives. Curricular documents may emphasize objectives that, on closer examination, are not effectuated in the actual lectures and laboratory courses. It is also possible that this particular curriculum may prove to be quite satisfactory. In that case, I can focus my research directly on the situation at hand. If not, the analysis in this section provides a general criterion for the construction of a situation more suitable for research.

2.4 The intended curriculum

2.4.1 Analysis of objectives

In the next sections I focus on the situation concerning education in organic chemistry at Utrecht University as it was at the beginning of this study in 1990. I will restrict myself to the first year of the curriculum. As I pointed out, this curriculum is followed by all chemistry students, and only by those students. During the period of my research, which stretches from 1990 to 1995, the curriculum did not change significantly.

A curriculum can be described from different points of view, with results that are not necessarily identical. The *intended* curriculum describes the curriculum as it is intended by faculty members and authors of educational material. I expect the intended curriculum to be compatible with the profile given in the previous section. The *realized* curriculum is the curriculum as it is seen and agreed upon by competent observers of the educational situation. It would be tempting to equate the ‘realized curriculum’ with ‘what really happens’. However, who can decide this? In truth, this description of the realized curriculum is a description from the point of view of the educational researcher, that is, from my point of view. Such a description should therefore be validated in some way. This is a question of methodology; I will address this issue in chapter 4. Finally, the *experienced* curriculum is the curriculum as it is experienced by those involved in the educational process. In this respect I could recount that students, teachers and the responsible faculty members, seem to be fairly satisfied with the curriculum. I have heard some moderate complaints about the cookbook character of the laboratory course, but the overall opinion seems to be positive. I did not commit a full-fledged satisfaction analysis, though. Such an analysis perhaps could have revealed that both students (who receive good grades) and teachers (who have heavy research obligations) have reasons not to bother each other too much. However, I think that the *quality* of education should not be evaluated using teacher or student *satisfaction*. Satisfaction does not guarantee quality. The aim of the curriculum is to prepare chemists who posses professional qualities, not chemists who were satisfied with their instruction. Consequently, I will not pay much attention to the experienced curriculum, but instead focus on the relations between what happens in professional chemistry and what happens in education.

In this section I describe the intended curriculum: the formal description of objectives, content, and organization in curricular documents such as the official student guide, the laboratory manuals and textbooks that are used in the first year.
According to the official student guide, the *Studiegids 1990-1991* (Faculteit, 1990), the first year is differentiated into nine subjects labelled "theory", which have familiar names such as Organic Chemistry, Physical Chemistry, and Structure & Bonding. These subjects are taught through *lectures* and *tutorials* in which smaller groups of students work on selected problems under supervision. Another set of subjects (such as synthesis, measuring, error analysis, safety) is dealt with in the *laboratory course*. The laboratory course is responsible for teaching "practical and social skills". The extent of the first-year curriculum is 1560 hours; 75 hours are devoted to the organic chemistry lecture course and tutorial; roughly 100 hours are devoted to organic chemistry during the lab course.
The student guide gives a description of all subjects. Organic chemistry is of course explicitly dealt with in the lecture course Organic Chemistry and in the related tutorial. It is possible that other subjects also pay some attention to organic chemistry, since in the description of certain subjects it is stated that "the relation with other subjects is indicated", although an elaboration of the nature of this indication is absent in the student guide.
The lectures in organic chemistry are given by a senior faculty member, usually a full professor in organic chemistry. The tutorials are supervised by teaching assistants. Both use John McMurry's *Organic Chemistry* (McMurry, 1988). In 1990, the lecture course dealt with the chapters 1-11, 14, 17 and 18. During tutorials students work on selected problems from the textbook; sometimes extra explanations are provided.

The student guide, describing the subject Organic Chemistry, mentions:

> ***Objective***
> The lectures provide the student with basic knowledge on organic chemistry. This basic knowledge is such, that he is sufficiently informed to successfully follow the other chemistry subjects, including the synthesis laboratory courses. The tutorials provide the students with the opportunity to learn to assimilate and handle the subject matter of the lecture course under expert supervision.
> ***Content***
> The lecture course deals with the following subjects:
> - physical and electronical properties of atoms and molecules, as far as is relevant for first year and second year organic chemistry.
> - the spatial structure of molecules.
> - common substance classes, such as alkenes, alcohols and ethers.
> - common reaction types, such as substitution, addition, elimination, including their reaction mechanisms. Knowledge of these mechanisms is necessary to understand the reactions of organic compounds.

The original, of course, is in Dutch. All translations of curricular documents into English are mine. I have tried to translate them as literally as possible. The results are not always very clear, but so, unfortunately, are the originals.
During the first year of the study, all laboratory work is organizationally integrated into one, all year course, called *Meten & Maken 1*, which means Measurement & Synthesis 1 (M&M1). This course comprises one to one and a half day each week. Its topics, subjects,

and organization are not directly related to any of the lecture courses. Concerning M&M1, the student guide mentions:

> *Objective*
> Learning to experiment, especially basic skills which are needed for chemical research. Acquaintance is made with a broad range of chemical topics, both in the area of learning to measure as well as in the area of learning to synthesize, isolate, and characterize substances.
> ***Content***
> - Knowledge of safety, error analysis, and phase theory (integrated lecture course/tutorial).
> - Analytical chemical techniques such as chromatography, potentiometry, spectroscopy (UV-Vis, AAS, etc.).
> - Synthesis of some inorganic and organic compounds, including such techniques as refluxing, extraction, distillation, crystallization etc.
> - Isolation of desired substances from biochemical systems (enzymes, lipids).
> - Measurement of physical-chemical quantities such as vapor pressure, conductivity, reaction rate.
> - Communication skills such as reporting and use of library.
> - An introductory course on computer usage (including the programming language PASCAL).
> - A small research project of own choice (group work).
>
> The substances and reactions to be studied are chosen in such a way that the relation with use in society is clarified.

As the student guide mentions, some minor lecture courses (error analysis, phase theory, and computer utilization) also take place during the laboratory course. The laboratory work itself consists of a series of 17 experiments, 4 of them being organic syntheses, evenly distributed over the year.

A senior staff member is director of the laboratory course, which is an almost full time occupation. He is assisted by another staff member.

Each group of about eight students is supervised by one teaching assistant (TA). Students perform the experiments either individually or in duos. TA's usually are either students in the final years of their study, or junior researchers. Occasionally, senior staff members carry out their 'teaching obligation' as a TA. TA's are sent to the laboratory course by the various chemistry departments; they are not recruited by the lab course management.

The laboratory course uses a manual (Derissen & Van Roon, 1990) that is written by the director and the assistant-director. This student manual often refers to commercially available laboratory manuals and textbooks, which students can consult in the laboratory's own library. Many experiments–and all the organic synthesis experiments–are based upon prescriptions that can be found in such books.

The student manual is accompanied by a teacher manual, which provides the TA's with excerpts from theory, instructions on how to handle laboratory instruments, data from literature, results to be expected, answers to questions posed in the student manual, and detailed chemical trouble shooting information for each experiment.

The student manual contains an introduction that elaborates on the objectives of the laboratory course. The following excerpts stem from this introduction:

> From the general objectives of the first year objectives have been derived for the first year laboratory course:
> 1. **Learning to experiment**
>
> The stress should be on:
> - to observe properly in self-conducted experiments;

> - to be able to indicate which purpose is served by the various parts, and how these relate to each other;
>
> (...)
>
> - to formulate the results decently.
>
> It is intended that certain skills and techniques, which are used regularly in experimental chemistry, will be learned. However, it is not the case that one must learn to employ all sorts of sophisticated devices and techniques; one should especially learn how to deal with current laboratory apparatus and learn the actions and principles that form the basis for specialization and broadening during the study.
>
> **2. Getting acquainted with a broad range of chemical topics**
>
> (...)

From these curricular documents it seems clear that the important objectives in the Utrecht intended curriculum are: *(1) learning to experiment; (2) learning basic knowledge; (3) learning basic skills; and (4) getting acquainted with chemical topics.* It is also clear that the aspects basic knowledge and basic skills, at least initially, are treated separately: the lecture course deals with basic knowledge, the laboratory course with basic skill. It remains possible, though, that, while learning these aspects, some integration occurs. Further analysis has to reveal this.

Of course, the situation at Utrecht University is a singular one. No other curriculum in the world will match it in all detail. However, I want to draw conclusions that reach farther than just Utrecht. Hence, I compared the Utrecht intended curriculum with the objectives of several other textbooks and lab manuals, to find that the intended objectives of the Utrecht curriculum largely agree with the intentions of other textbook authors (Atkins, 1987; Brewster, Vanderwerf, & McEwen, 1977; Cram & Hammond, 1959; Fieser & Williamson, 1987; Holleman, 1955; Hünig, Märkl, & Sauer, 1979; Mann & Saunders, 1964; March, 1985; McMurry, 1988; Pavia, Lampman, & Kriz, 1982; Roberts & Caserio, 1965; Salemink & Biessels, 1980; Schumm, 1987; Skoog & West, 1982; Streitwieser & Heathcock, 1985; Ternay, 1976; Vogel, Furniss, Hannaford, Smith, & Tatchell, 1989; Williamson, 1989).

I will illustrate this with some examples. The introduction of Williamson's Macroscale and Microscale Organic Experiments (Williamson, 1989) states:

> [The objective of this book is] to introduce undergraduates to the basic techniques of the organic laboratory in preparation for carrying out a wide range of meaningful experiments that exemplify the principles of organic chemistry.

This can be seen as a very concise combination of the same four objectives. "Introduce to basic techniques" is the equivalent of 'learning basic skills'. "Exemplify" and "a wide range of meaningful experiments" agree with 'getting acquainted with chemical topics'. "Principles of organic chemistry" corresponds with 'basic knowledge'. The whole sentence, perhaps, can be interpreted as meaning 'learning to experiment'. However, "carrying out experiments" is not exactly the same as 'learning to experiment'. Maybe the latter can be achieved through the first, but this still needs justification. I will deal with this question below.

The objectives 'learning basic knowledge' and 'getting acquainted with chemical topics' can also be found in McMurry's textbook, in use in Utrecht. Although this book does not state its objectives, the preface contains many remarks that are analogous: "providing an accurate and up-to-date view of organic chemistry"; "explaining the fundamental mechanistic similarities of reactions"; "help students learn to organize and work with the large body of factual information that makes up organic chemistry"; and "this book contains a wealth of material helpful for learning organic chemistry" (McMurry, 1988), pp. iii-v).

It can be inferred that the Utrecht curriculum corresponds with many other curricula in the world with respect to the objectives, and perhaps also with respect to contents and organization. However, it is also clear that this intended curriculum dissents from the profile I drew in the previous section. It seems that the professional qualities are dealt with in isolation from each other. The lecture course deals with 'basic knowledge' that is necessary to "successfully follow the other chemistry subjects, including the laboratory courses". This is an internal educational target. Professional research qualities are not mentioned nor are situated aspects. The laboratory course mentions 'learning to experiment', which could be the combination of professional qualities with situated aspects. However, the objective is specified as "basic skills that are needed for chemical research", which can also imply that skills are taught as decontextualized manipulation. It remains to be seen whether the laboratory course agrees with the previous section's profile. It is a problem that clear definitions or descriptions of words like 'basic', 'getting acquainted with', 'principles', 'topics' and 'properly' are lacking.

2.4.2 Analysis of content

Generic terms like 'basic skills', 'basic knowledge', and 'chemical topics' mean little without an indication of content. 'Learning to experiment' is more process-like, and needs to be fleshed out differently. I will deal with this objective in the next section.

Basic knowledge

The content corresponding with 'learning basic knowledge' can be derived from the chapters in McMurry that are treated in the lecture course. These are summarized in Table 2.1. Other textbooks cover approximately the same material as McMurry, using approximately the same organization. The choice of chapters at Utrecht University does not appear to be controversial. An attempt is made to provide a representative picture of organic chemistry.

Listing contents in terms of titles of chapters is not very efficient. Even introductory textbooks like McMurry's Organic Chemistry contain more than a thousand pages, and have many chapters. Clearly, without some meaningful organization, nobody, let alone a novice, would be able to learn the material. I therefore suggest to speak about contents in more comprehensive terms. In his introduction McMurry writes:

> This book uses a dual functional-group/reaction-mechanisms organization. The primary organization is by functional group, beginning with the simple (alkenes) and progressing to the more complex. Within this primary organization, however, heavy emphasis is placed on explaining the fundamental mechanistic similarities of reactions. [...] Many students attach great importance to the lead-off reaction in a text, because it is the first reaction they see and it is discussed in such detail. I have

chosen a simple polar reaction - the addition of HBr to an alkene - as the lead-off to illustrate the general principles of organic reactions.

Table 2.1 *Basic knowledge in terms of McMurry's chapter titles*

1	Structure and Bonding	8	Alkynes
2	Bonding and Molecular Properties	9	Stereochemistry
3	The Nature of Organic Compounds: Alkanes and Cycloalkanes	10	Alkyl Halides
4	Stereochemistry of Alkanes and Cycloalkanes	11	Reactions of Alkyl Halides: Nucleophilic Substitutions and Eliminations
5	An Overview of Organic Reactions	14	Conjugated Dienes and Ultraviolet Spectroscopy
6	Alkenes: Structure and Reactivity	17	Alcohols and Thiols
7	Alkenes: Reactions and Synthesis	18	Ethers, Epoxides, and Sulfides

This organization clearly shows in titles as 'Reactions of Alkyl Halides: Nucleophilic Substitutions and Eliminations'. It appears that McMurry organizes content with three principles: (1) Substances are categorized in relatively few classes, each having the same functional group. Having the same functional group implies similarities in chemical and physical behavior, and in molecular structure. Examples: alkanes, alcohols, amines, carbonyl compounds. (2) Reactions are generalized into classes too. The instance of two particular substances that react to a particular product can be presented as two examples of substance classes that react following a general pattern towards an example of another substance class. Examples: alkylation of aromatic compounds; esterification. (3) Reactions can also be generalized with respect to mechanism. Esterification and hydrolysis are examples of aliphatic nucleophilic substitution.

Almost all textbooks use an organization based on these three principles, and it seems to me that these are the principles that lab courses use to exemplify and illustrate organic chemistry: they make a selection of those substance classes, reaction classes and reaction mechanisms that are considered to be representative of organic chemistry.

Basic skills

Table 2.2 *Basic laboratory techniques of organic chemistry*

Heating and cooling
Adding solids, liquids, and gasses
Mixing and stirring
Refluxing
Filtration
Extraction
Distillation (normal, vacuum, steam)
Crystallization
Chromatography (TLC, GLC, and column)
Spectroscopy (UV/VIS, IR, NMR)
Determination of physical constants (boiling point, melting point, refraction index)

Proceeding from 'learning basic techniques of organic chemistry' to its contents proves not to be very difficult. The techniques mentioned in Williamson's book are listed in table 2.2. Almost all these techniques are dealt with in the Utrecht laboratory course. Other books pay attention to the same techniques. There seems to be little dispute about basic skills.

Getting acquainted with chemical topics

Which contents belong to the objective 'getting acquainted with chemical topics'? This is a difficult one, since both 'topic' and 'getting acquainted with' are inherently vague. Anything from using a beaker to chemical warfare can be called a chemical topic. I suppose that this objective symbolizes something of the context in which chemists work. Restricted to the laboratory, chemists can be seen to determine molecular structures, measure the kinetics of reactions, analyse the composition of natural materials, etc. But these 'topics' themselves often are part of a bigger world: chemists prepare medicines, food additives, detergents, etc. It seems that the curriculum should illustrate this. Chemists resent it that the general public is oblivious to the benefits bestowed on them by chemistry. People eat their food, use their medicines, do their laundry and watch television without knowing the world of chemistry behind these daily-life items. Quite the contrary, they associate chemistry with pollution, danger, and waste. Chemistry students should become more literate. So they do not just measure for measurement's sake; they measure the fatty-acid composition of olive oil. Similarly, they do not just synthesise random substances, but they make an analgesic like aspirin, or a fabric dye. From the more restricted point of view of the profession, each department–organic chemistry, electrochemistry, biochemistry, kinetics, etc.–has its own experiments. Within organic chemistry, topics include isolation, synthesis, molecular structure, reaction mechanisms, catalysis, and many more, which are all present in the lab course as a whole.

A problem for any lab course is that textbooks and books on laboratory experiments do not know constraints: they contain as many topics as the publisher approves of. This means that all treat the whole field, because otherwise people would by another book. It is up to the curriculum, then, to make choices. From the professional point of view, it is evident that the Utrecht curriculum does not try to be up to date with respect to current research. The organic syntheses that are part of the curriculum are classic experiments, such as the synthesis of aspirin and the nitration of toluene. A relation with society is made by the inclusion in the text of a section explaining the role of the product in society. Aspirin is an analgesic, azobenzene is a dye, *p*-chlorobenzoic acid is a conserving agent, etc.

So far, the intended curriculum seems to be internally consistent and undisputed. This is partly because I have paid little attention to the objective 'learning to experiment'. I will now deal with this objective in more detail.

2.4.3 Learning to experiment?

To me, 'learning to experiment' is the most important objective, since it could comprise both the professional qualities needed to do research and the situated aspects determining what to do and why. This objective would require a combination of knowledge, skills, and topics. Analyzing this objective implies analyzing how the curriculum tries to *integrate* these aspects, since they initially are dealt with separately.

Textbook and lecture course

The student guide promises that the lecture course will enable the students to deal with the lab course successfully. The lab course, in its turn, has as its most important objective 'learning to experiment'. In which way does the textbook try to be of help in learning to experiment? McMurry's Preface is promising. Here he writes:

> Organic synthesis is emphasized as a teaching device to help students learn to organize and work with the large body of factual information that makes up organic chemistry. Two sections (...) clearly explain the thought processes involved in working synthesis problems.

I will now critically examine the role of the textbook in learning to experiment. Textbooks present a survey of the established facts, that is, they present the *results* of former research. From this point of view, it is not necessary to mention the original research context: the questions, assumptions, hypotheses, problems, and methods of the original research context have disappeared from the text (Cooley, 1991).

Science aims at making facts: Fleck (Fleck, 1979) and Latour (Latour, 1987; Latour & Woolgar, 1986) show how experimental findings such as taints in a Petri dish or lines on a chromatogram gradually are transformed into irrefutable statements concerning facts of nature. The process starts with private lab notes, continues with journal articles and review articles, and comes to a temporary end in educational textbooks, which do not anymore contain the references to the original literature. The highly structured presentation of the facts in a seemingly logical order in these books suggests that the discoveries have been made and can be made using a priori argumentation. Every scientist knows that this is seldom the case, although it can be difficult to escape from its charm (Joling, 1993). Many chemical discoveries have their origin in tentative or even provocative assumptions and conjectures, combined with a laborious trial and error process in the laboratory. "The many brilliant and novel synthetic schemes, often of compounds of great structural complexity, which have been accomplished in the past are attributable largely to the intuitive skills of the research chemist" (Vogel, et al., 1989). When a problem has been solved, it is often possible to provide a rationale, but only with hindsight. Through textbooks and lecture courses, students can learn to reproduce the facts and the way chemistry structures these facts using concepts such as functional group and reaction mechanism. However, to create new facts more is needed than knowledge of bare, decontextualized facts. "In practice, scientists proceed partly by rationalization (based on their theoretical understanding) and partly by intuition rooted in their tacit knowledge of how to do science (their connoisseurship)" (Hodson, 1992a).

Textbooks are printed on paper. They show the *paper* part of chemistry. This implies that compounds are represented by names and formulae. This greatly improves the comprehensibility of organic chemistry. It is obvious that it is far easier to categorize compounds with formulae than with their perceived properties. This advantage, however, is gained at some cost: chemistry is about real substances and reactions and not only about their representations. The ability to represent substances with particular molecular formulae, space-filling models, etc. is itself a result of research. From this point of view, it is questionable whether transfer of 'basic knowledge' in the form of such representations is suitable to prepare students for research aiming at the development of such representations. Students may be completely unaware that what they learn is not brute fact, but human construct.

Ultimately, organic chemistry is about *phenomena*; names and molecular structures are chosen to represent chemical behavior. For example, the compound salicylic acid contains a hydroxy group as well as a carboxylic acid group. The hydroxy group, if it has phenol-like properties, can also have acidic properties. The name of the substance ('acid') suggests to emphasize just this acidic character. However, in the conversion to aspirin, salicylic acid is esterificated, which means that substance behaves as an alcohol. The substance could thus be called an alcohol as well as an acid. This reaction phenomenon could perhaps be predicted by an experienced chemist, but a novice could be confused by the inappropriate name.

Reactions that appear logical on paper may be disproved by the empirical facts. The ability to solve synthesis problems on paper should not be equated with the ability to synthesize these compounds in the laboratory: "The inscriptions of routes on paper can never replace the actual attaining of crystals in a bottle" (Turner, 1976). However, textbooks hardly pay attention to laboratory techniques, with the exception of methods for the determination of structure. The aim of this is not to help students to master these skills; rather, the aim is to discuss a new class of substances that can be investigated with this technique. An example is the combination in one chapter of ultraviolet spectroscopy and conjugated dienes. There is no intention to treat 'basic knowledge' in relation with the laboratory methods necessary to obtain knowledge.

Chemistry is underdetermined by theory, and only empirical evidence can decide between alternatives that are theoretically plausible (Van der Vet, 1987). *The textbook way of dealing with the facts can lead to a misunderstanding of science, especially concerning the instrumental nature of scientific theory in research.* Students learn to reproduce the facts and the explanations, but they should also learn *to establish* facts, learn *to explain*. Textbooks and lecture courses look backwards, to what has been achieved in the past. This is not sufficient to prepare students for what they have to achieve in the future.

McMurry's 'practice problems', therefore, cannot be seen as a tool for learning to experiment. They are a tool for learning the facts. McMurry himself states (p. 246):

> In this book, too, we will often devise syntheses of molecules from simpler precursors. The purpose, however, is purely pedagogical. The ability to plan workable synthetic sequences demands a thorough knowledge of a wide variety of reactions; it also requires a practical grasp for the proper fitting together of steps in a sequence such that each reaction does only what is desired. *Working synthesis problems is an excellent way to learn organic chemistry.*

This boils down to the statement that, to solve synthesis problems, one has to posses textbook knowledge, and that working exercises is an excellent tool to achieve this goal. In other words, an *internal* educational goal is justified with another purely *internal* goal. Whether the solutions are 'workable' in practice is not an issue. They cannot even be verified, since McMurry does not refer to primary literature.

I do not dispute that textbook knowledge is useful and necessary. Nor do I want to suggest that any lecturer or textbook author is thinking that textbook knowledge is in itself sufficient for becoming a good experimental chemist. However, I want to challenge the implicit suggestion that learning facts through textbooks is taking a step towards 'learning to experiment'. Many chemistry educators seem to think so, since it is quite normal that the lecture course precedes the laboratory. Sometimes it is even required that students have passed an organic chemistry test (and other lecture course tests) before they are allowed to take the laboratory course. Textbook knowledge is seen to be a necessary prerequisite for experimenting. However, Bowen (Bowen, 1990) showed that even advanced graduate students, while solving complicated paper and pencil synthesis problems, rarely take into account which routes will be possible in the laboratory. I will return to this theme in chapters below, where I will argue that students are often not able to apply textbook knowledge successfully.

I conclude that 'learning basic knowledge' is insufficient preparation for 'learning to experiment'. This basic knowledge is not *situated knowledge* and hence is not clearly related to the professional context.

The laboratory course

My first impression of the objectives for the laboratory course was quite satisfactory. 'Learning basic skills' is undisputed, and 'learning to experiment' seems to be in line with the principal aim of scientific chemistry education. The latter objective is elaborated in the introduction to the student manual. Here it says that students should "be able to indicate which purpose is served by the various parts, and how these relate to each other". This, however, is a strange sentence. Someone who is experimenting is in control of the activities, and the purpose and relations of the various parts cannot be unclear. I interpret this sentence in the sense that the authors of the text do not discriminate between *experimenting*, that is, the activity to empirically find an answer to a problem, and the activity of *carrying out experiments* in the cookbook sense, that is, following detailed instructions. To me, these are different things. Students who do not make their own choices but instead receive a set of instructions, are not experimenting. What they do, however complicated it is, has little to do with experimenting, except the semblance of the words in language.

Cookbook experiments are completely controlled: the outcomes are known in advance; students chose neither their own techniques nor their methods; nor do the students determine the nature of the problem (Meester & Maskill, 1993). In contrast, in 'experimenting', the experimenter determines the problem; tries to find adequate methods and techniques; and the outcomes are not known in advance. So, the word 'problem' has a different meaning in both situations, too. In carrying out experiments the problems have little or no resemblance to the types of problems that occur in experimenting. The difficulties within cookbook experiments have to do with the technical manipulation of the equipment necessary to carry out the prescriptions, and with reproducing the correct causal explanations. In experimenting, the difficult part is to pose questions and to determine which methods and experiments may provide answers to these questions. The ability to manipulate is a prerequisite, whereas theoretical explanations and justifications are possible only after the experiments have been conducted and interpreted.

It can be concluded that the manual makes the unwarranted inference that one can learn to experiment by carrying out experiments. If this is assumption is not true it is unclear in what respect the course prepares students for doing research.

An analysis shows that the laboratory course contains four organic synthesis experiments. All employ detailed prescriptions, which the students have to follow. The rationales are provided beforehand in the manual, or have to be looked up in textbooks.

Without doubt, the single most important objective of the laboratory course is 'learning basic skills'. This becomes especially clear if the experiments are analyzed regarding the techniques present and regarding reactions, mechanisms, and substances, as I have tried to do in table 2.3. The experiments show representativity with regard to laboratory techniques. The experiments show some variety, but certainly not representativity, concerning substance classes. Relations between basic skills and 'principles of organic chemistry' appear to be random, as is exemplified by the occurrence and order of mechanisms.

Table 2.3 *Mechanisms, substances, and techniques*

Mechanism	**Substances (classes)**	**Techniques**
Organic synthesis 1: Aspirin		
second order nucleophilic substitution (esterification)	acetic anhydride (carboxylic derivative salicylic acid (alcohol) sulfuric acid aspirin (ester)	refluxing crystallization filtration drying melting point infra-spectroscopy
Organic Synthesis 2: Chlorobutane or bromobutane		
second order nucleophilic substitution	2-butanol or 1-butanol (alcohol) hydrochloric acid with zinc chloride; or hydrobromic acid 2-chlorobutane or 1-bromobutane (alkyl halide)	refluxing distillation extraction gas chromatography refraction index
Organic Synthesis 3A: P-chlorobenzoic acid (step 1&2)		
aromatic electrophilic substitution (nitration) reduction	nitric acid sulfuric acid toluene (aromatic compound) p,o,m-nitrotoluene (nitro aromatic compound) tin p-nitrotoluene hydrochloric acid p-toluidine (aryl amine) sodium hydroxide diethyl ether (ether)	adding and stirring cooling extraction and drying vacuum distillation freeze crystallization gas chromatography refluxing steam distillation rotation vaporization crystallization melting point infrared spectroscopy
Organic Synthesis 3B: P-chlorobenzoic acid (step 3&4)		
diazotation + Sandmeyer reaction oxidation	p-toluidine (aryl amine) hydrochloric acid sodium nitrite cuprous chloride p-chlorotoluene (aryl halide) potassium-permanganate hydrochloric acid sodium metabisulfite p-chlorobenzoic acid (aromatic carboxylic acid)	adding and stirring cooling and heating steam distillation extraction and drying vacuum distillation refraction index gas chromatography infrared spectroscopy refluxing filtration crystallization melting point

Organic Synthesis 4A: Iodoform		
electrolytic oxidation	potassium iodide sodium carbonate carbon dioxide ethanol iodoform	electrolysis gas addition stirring heating filtration drying melting point infrared spectroscopy
Organic Synthesis 4B: Azobenzene		
electrolytic reduction	potassium iodide sodium carbonate carbon dioxide ethanol iodoform	electrolysis cooling and stirring vaporizing extraction rotation vaporization column chromatography crystallization melting point infrared spectroscopy

It is not clear which criteria have been used to produce this particular selection, but clearly not McMurry's organizer: "I have chosen a (...) reaction (...) as the lead-off to illustrate the general principles of organic reactions". It seems that on the level of basic skills and basic knowledge the various parts of the curriculum are unrelated. The lab course, for example, contains experiments on aromatic electrophilic substitution, whereas the first year lecture course does not treat aromaticity. Rather, the choice of the prescriptions seems to be based entirely on the laboratory techniques. Also apparent is an order in increasing complexity of manipulation: normal distillation precedes vacuum distillation which in turn precedes steam distillation; filtration precedes extraction, etc. It is the equipment that becomes more complicated through the year; however, this is not driven by a demand to obtain ever better chemical results. Neither is it the need to make a special product with a specific purity that determines the choice of techniques, rather, it is the other way round: a specific synthesis is sought to match a certain technique.

This exclusive attention to manipulation threatens the validity of the experiments. For example, Organic Synthesis 3 is supposed to be a multistep synthesis. A multistep synthesis is characterized by the fact that the product of a first step is used for a second step. In this experiment, however, students start the second step with fresh reagents from the stock. When they would use their own products, the second reaction would fail too often and the students would not get acquainted with the final techniques. In this way, a specific objective–learning to manipulate–is attained, whereas another, more important objective–learning to get a good chemical result–is neglected.

The Nobel laureate Corey wrote in this respect that synthesis usually is taught "by the presentation of a series of illustrative (and generally unrelated) cases of actual syntheses. Chemists who learned synthesis by this 'case' method approached each problem in an ad hoc way. The intuitive search for clues to the solution of the problem at hand was not guided by effective and consciously applied general problem-solving techniques" (Corey & Cheng, 1989).

I therefore conclude that the lab course at best promotes 'learning basic skills'; contributions to 'learning to experiment' are accidental by-products that are not monitored by the curriculum.

Evaluation of the existing situation

The lecture course approximately meets its own standards, mainly because these are not defined as preparation for research but as preparation for other courses. It provides students with basic knowledge. It enables the students to pass the tests, and probably helps students to cope with other subjects. It is unlikely, though, that the lecture course will be of concrete help for the laboratory course, since it does not prepare for experimenting. The laboratory course chooses topics and substances not dealt with in the lecture course. The lab course contributes through its choice of compounds and reactions to students' basic knowledge. It certainly pays attention to basic skills, albeit in a decontexutalized sense. *However, both courses do not contribute explicitly to 'learning to experiment'.* They lack attention to the situated aspects necessary to understand knowledge and skills in such a way that research becomes possible. "The focus on 'passing the lab' and 'failing the course' is what is emphasized, not the enterprise of science. A two-faced nature of science has dominated science education practice during the 20th century: science as content and product versus science as inquiry and process. School science, which focuses almost exclusively on the content of science, presents an incomplete representation of science" (Costa, 1993).

The lecture course and the laboratory course are unconnected. The first is called 'theory', the second 'practice'. I wonder whether such a self-imposed separation should be taken for granted, since it is non-existent in scientific research. Research aims at the creation of facts and theories through practical investigation of theoretical hypotheses. This dual character of science is not recognized by the curriculum. Verdonk draws a similar conclusion about chemistry education: "Inconsistencies are noticeable, such as: (i) the isolation of scientific results from scientific questions; (ii) prescription instead of design of laboratory work; (iii) calculations only to test skills; and (iv) presentation of models as absolute facts" (Verdonk & Lijnse, 1993).

This analysis of the intended curriculum makes clear that it is unlikely that there is an explicit relation between students' learning to experiment in organic synthesis, and teaching. The present curriculum therefore probably is unfit to conduct educational research on how students learn to experiment.

2.5 The realized curriculum: the case of aspirin

The analysis of the intended curriculum revealed that it is not internally consistent and that it does not seem to prepare explicitly for the profession. If this is true, it must be visible in the realized curriculum. In this section, I therefore analyze one of the experiments more closely, focusing on the way basic skills, basic knowledge, chemical topics, and learning to experiment are dealt with, both in themselves and in relation with one another.

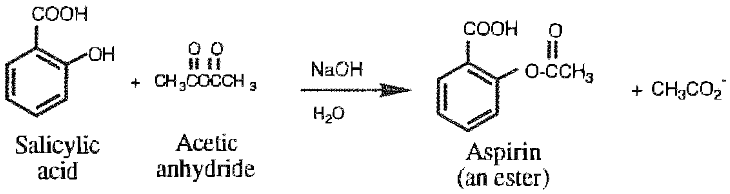
The experiment is called 'Organic Synthesis I: Esters'. It is one of the first experiments in the course, and the first organic synthesis. In this experiment, students have to make an amount of *aspirin*, using a prescription from literature. This synthesis is described in many laboratory manuals, and probably carried out in lab courses all over the world. In the Utrecht version, the students read a four page text from their manual, consisting of (1) the assignment ('prepare 13 g aspirin'); (2) some general remarks about organic synthesis; (3) references to textbooks in which to look up the prescription and the reaction equations; (4) some information on crystallization; (5) remarks about what will have to be discussed with the teaching assistant before starting with the preparation; and (6) information about how to write the report.

Prescription and information provided

The Dutch secondary school National Chemistry Assessment requires students to know the reaction equation of the normal ('Fischer') esterification; most textbooks give the acid catalyzed reaction of ethanol and acetic acid as an example. The aspirin synthesis will be unknown to the students.
They are supposed to look up the prescription in Vogel's *Textbook of Practical Organic Chemistry* (Vogel, et al., 1989). The prescription runs as follows:

> **Conversion to acetylsalicylic acid** (*aspirin*). Place 10 g (0.725 mol) of dry salicylic acid and 15 g (14 ml, 0.147 mol) of acetic anhydride in a small conical flask, add 5 drops of concentrated sulphuric acid and rotate the flask in order to secure thorough mixing. Warm on a water bath to about 50-60 °C, stirring with a thermometer, for about 15 minutes. Allow the mixture to cool and stir occasionally. Add 150 ml of water, stir well and filter at the pump. Dissolve the solid in about 30 ml of hot ethanol and pour the solution in about 75 ml of warm water; if a solid separates at this point, warm the mixture until solution is complete and then allow the clear solution to cool slowly. Beautiful needle-like crystals will separate. The yield is 11 g (85%). The air-dried crude product may also be crystallised from ether-light petroleum (b.p. 40-60 °C).

There also is a reference to McMurry's Organic Chemistry, in which the students can find the following reaction equation (p. 759). The aspirin synthesis is in a chapter of the textbook not dealt with in the lecture course:



The manual provides 'remarks' regarding synthesis:

> ***Remarks regarding the synthesis of a desired product***
> In general, there are several alternative reaction pathways which lead to the desired product, for example:
> carboxylic acid + alcohol → ester + water
> carboxylic acid chloride + alcohol → ester + water
> carboxylic acid anhydride + alcohol → ester + water
> The road to be chosen depends upon many aspects, for example:
> -cost and availability of the reagents
> -avoiding undesired side reaction or side products
> -favourable reaction conditions (temperature, pressure, solvent, etc.)

-higher yield
-safety, simplicity, time.

When the pathway is chosen, it is in synthesis in general possible to distinguish the following stages:

a. Adding the reagents to each other

This can be done in one (depends on the amount of heat generated), either in a solvent or not, with or without stirring, heating, etc. etc.

b. Formation of the desired product.

Care should be taken that the reaction proceeds fast enough, and comes sufficiently to completion. Influencing the equilibrium and/or the reaction rate by way of choosing excess amount, temperature, catalyst, etc. plays a role.

A product that can be withdrawn from the reaction mixture (gas evolution or precipitation) can be favourable.

c. Isolation of the crude product.

When the product is formed, it generally has to be separated from the side products, solvent and excess or unreacted reagents. Techniques such as filtration, extraction, etc. are commonly used. Drying (extraction of water) also can be counted among these. In general, the product will not be completely pure in one time. Consequently, a next step follows:

d. Purification of the crude product.

This has to be continued till the desired purity has been reached (this never is 100%, but depends on the objectives for using the product).

Techniques such as crystallization, fractionated distillation, chromatography are often employed.

e. Characterization of the final product.

It is always necessary to verify if the product meets the desired specifications. A wide range of physical and chemical analysis techniques can be used, ranging from the determination of macroscopic parameters such as melting point or refraction index till the use of complicated instrumental techniques as NMR; also quantitative analysis using titration, spectrophotometry, etc. etc.

Learning to experiment?

The following analysis is based on observations of the experiment and on discussions and informal interviews with students, teaching assistants and the director of the laboratory course. The methodological validity of this approach is discussed in chapter 4, where I will discuss questions concerning methodology relevant for the entire study.

The techniques featuring in this synthesis (adding, stirring, heating, filtration, crystallization) are not very complicated from a manipulation point of view, which makes the experiment suitable to start with. According to the director this had been the most important reason for choosing this experiment: it is a 'learning basic skills' experiment. Another reason for choosing this synthesis is the 'getting acquainted with chemical topics' objective: aspirin symbolizes the relation between chemistry and society. Still, the background assumption is that students 'learn to experiment'.

Since this is a prescription experiment, it is a test case for the assumption that students can 'learn to experiment' by 'carrying out' this prescription. The 'remarks on synthesis' section of the manual suggests that the 'learning to experiment' objective is indeed being pursued, since this text deals with the choices to be made in synthesis in general. Otherwise, the section could have been left out. However, in this experiment, a context of inquiry seems absent. Students do not decide which product to make or which problem to investigate, nor do they choose methods or techniques. The outcome of the experiment is known in advance.

The strategy chosen is to treat 'theory' separated from 'practice': the reaction equation and the 'remarks' are not integrated with the prescription. A first question is whether integration takes place during the experiment.
This strategy seems to backfire almost immediately: according to McMurry, the reaction is base catalysed, whereas Vogel's prescription is acid catalysed. During the introductory discussion, students who have copied the base catalysed version have to replace the equation. Fortunately, this does not alter the lab actions themselves. Little or no time is devoted to the 'remarks' during such prelab discussions, which focus almost entirely on how to carry out the prescriptions: what is a conical flask?; how to stir?; how to filtrate?; how to crystallize? The skills appear to be central. The remarks remain largely unread and undiscussed.

Since students do not really experiment, it is difficult to assess 'learning to experiment' directly. I suggest to assume, for the sake of this analysis, that the objective is advanced when the students become aware of relations between theory and practice in this experiment. In the analysis below, I follow the 'remarks'.

Choice of reaction pathway

Clearly, the choice of a pathway is made by Vogel. This reaction is an esterification, but not a very typical one. The typical textbook esterification reaction has an alcohol and a carboxylic acid as starting reagents. In this reaction, however, acetic anhydride is used instead of acetic acid. Empirically, acetic acid is found to be almost unreactive towards salicylic acid. In such cases, the more reactive anhydrides can be used. The acid chloride probably is not used because of its more hazardous properties. The reaction is almost as fast as salicylic acid dissolves, which makes it one of the faster reactions in organic chemistry. A reaction with carboxylic acid would have produced water as a side product. Water can hydrolyse aspirin, and this is avoided: the reaction between salicylic acid and acetic anhydride generates acetic acid as a by-product. The acetic acid will be harmless, since a reaction with salicylic acid would again produce aspirin. McMurry's base catalysed reaction seems less suitable for synthetic purposes, since both water and the hydroxy ion can hydrolyse the product. The acetate ion that is formed could redress this, but it is a weaker nucleophile than OH^-. McMurry's equation even seems irrational, since the previous page the book states: "acid anhydrides react with water to form acids" (p. 758).
However, students are unaware of these rationales. Many of them do not even know that this reaction is an esterification. They cannot give arguments for using acetic anhydride, except that the prescription says so. They cannot give arguments for choosing acid catalyzed above base catalyzed. Some students do not notice that the two books use different catalysts. They also do not notice that salicylic acid reacts as an alcohol and not as an acid.

Adding the reagents and formation of the product

The description specifies the amounts of salicylic acid and acetic anhydride using mass units. The amounts in mole between the brackets contain a typo: 10 g salicylic acid corresponds with 0.0725 mole. This means that a twofold excess of acetic anhydride is used. Organic chemists prefer homogeneous reactions in the liquid phase. A liquid medium is able to disperse heat effects quickly and safely, and provides optimum contact between reagents. Since salicylic acid is a solid, a solvent is needed. Acetic anhydride, which is the other reagent, is a liquid and it happens not only to react with salicylic acid, but also to dissolve it. When excess acetic anhydride is used no other solvent is needed. Hence, a potential extra separation problem is avoided. Excess acetic anhydride guarantees that little salicylic acid will be left. This is to be preferred, since removal of salicylic acid from aspirin is harder than removal of excess acetic anhydride. Some textbooks suggest that the reaction is an equilibrium (Pavia, et al., 1982). If that is true, excess acetic anhydride will also reduce the amount of salicylic acid present in the equilibrium mixture.

Heating ensures that all salicylic acid quickly dissolves; it also increases the reaction rate. Warming on a water bath prevents the medium to reach a temperature in which aspirin may decompose. On slowly cooling down, aspirin precipitates without enclosing impurities such as traces of salicylic acid. Unreacted salicylic acid, when present, will remain dissolved since its concentration is small.

Mechanistically, the esterification reaction is a second order nucleophilic substitution. Such reactions on carbonyl compounds often are acid-catalyzed. Hence the presence of concentrated sulfuric acid. This specific acid is used because it does not contain any water, as do hydrochloric acid and nitric acid. Water-containing acids could react with acetic anhydride, and water could hydrolyse aspirin. Unfortunately, hardly any student notices that a twofold excess of the anhydride is used, let alone that they know for what reason. As said, many students do not know that this reaction is an esterification, they do not know that it is a nucleophilic substitution, and the only argument they can give for adding sulfuric acid is, again, because the prescription says so.

Isolation and purification of the crude product

Water is added for several reasons. The product, aspirin, hardly dissolves in water, and will precipitate almost completely. Acetic acid and sulfuric acid are soluble in water, and can be removed in this way. Acetic anhydride is not very soluble in pure water, but dissolves rather well in a mixture of water and acetic acid. Remaining acetic anhydride, since it is a liquid, can be washed and sucked away during the Büchner funnel filtration. In this way, all impurities are removed, leaving aspirin behind. The only drawback is the potential hydrolyses of the product by water. For that reason, cold water should be used. In fact, this procedure is wonderfully efficient: separation and almost complete purification in one step, without effort.

Again, students cannot explain this. Many are even unable to give this activity a proper name, like separation or purification, suggesting that they do not know that they are trying to get rid of impurities. This becomes visible in the way they handle the Büchner funnel filtration: instead of adding and stirring the water through the precipitate when the pump is off, they keep applying suction.

Crystallization is prescribed. However, it can be doubted if this will add much to purity, which already is quite high. In fact, most student products were purer *before* crystallization. Students are not aware of the potential hydrolysis reaction. They add water that is not cold enough to a mixture that still is fairly warm. During crystallization, the aspirin solution is often kept boiling for some time. Over-all, more salicylic acid is introduced in this way than is removed.

Apparently, crystallization is present as part of the 'learning skills' objective, but students do not really learn much about the relations between goal and activity. In this case, there is no 'desired purity' specified. Nor is there an 'objective for using the product': the product is thrown away.

Characterization

Nobody really doubts that the product is aspirin. Consequently, techniques like IR and melting point are, again, applied in the context of learning skills, and not in the context of learning to experiment. The information is not used to evaluate the synthesis procedure, but to demonstrate the technique itself. If anything is evaluated, it is the students' ability to execute the procedure.

Basic skills, basic knowledge, chemical topics

What has been said above about the Büchner funnel filtration is also true of the other techniques. Since there is no clear relation between doing something and its rationale, the technique remains a form of decontextualized manipulation. It is somewhat strange to teach a purification technique on a substance that already is almost pure. Students do not learn to apply the techniques to solve a problem, or to answer a question. They reproduce actions, which, in this specific case, lead to the desired result. Thus, even 'learning basic skills', as the single most objective in this experiment, is subjected to the goal of obtaining a product. The students, it can be said, learn to make aspirin instead of 'basic skills'.

The chemical knowledge and theory in this experiment hardly are 'basic' from the chemical point of view. Even the objective of illustrating important reactions and substance classes is not met in this experiment. Esterification, alcohols, and carboxyl compounds are important, but this experiment is not very representative for these topics: the alcohol is an acid, the acid is an anhydride, and, instead of forming the equilibrium mixture typical of esterifications, this reaction already has an almost 100% yield before purification. The reaction mechanism, nucleophilic substitution, receives no attention. There is no relation with the 'principles of organic synthesis'. The theory on organic synthesis presented in the 'remarks' is not related to practical decision making. Since students do not need it to perform the experiment, they read this section only superficially, if at all.

The prescription and the reaction equation are written in a matter-of-fact-like language. There is no trace of doubt or difficulty, or of a context of inquiry. It took chemists years of research to develop procedures like this, and they are now carried out in freshmen laboratory courses as a matter of routine.

Aspirin symbolizes chemistry's impact on society. However, in this experiment, society is far away. The aspirin is not used, not made for use and not evaluated from a user's point of view. The relations between chemistry and physiology (what makes aspirin such an efficient pain-killer?) receive no attention.

A few months later, the students have forgotten many details of the procedure: names like acetic anhydride and esterification, the formulae, activities like adding sulfuric acid or washing with water, the use of an excess. Students still have vivid images of white powders and colourless liquids, which were mixed and heated and stirred and filtrated, and they remember that the procedure was highly successful: they had made aspirin and they had received a high mark.

It seems to me that there even might be a correlation between the elegance of the procedure and the lack of understanding. Since students need not worry about why and wherefore, they can focus exclusively on the how. *This is exactly the cookbook problem:*

"The fault of many organic experiments seems to be that there are no questions asked and no thinking done, only instructions given to allow students to obtain products whose properties are matched to known values". No questions need to be asked–except for the how-do-I-do-this type of question–and no thinking needs to be done to obtain excellent chemical results and, consequently, high marks. *There is no need to understand.* In this cookbook experiment, the goal is to make a chemical substance and not to achieve understanding. Every element–the pathway, the reaction conditions, the purification techniques, etc.–is motivated by this goal. All other goals, such as learning basic skills, learning basic principles of organic synthesis, and learning to experiment will be attained, if at all, only indirectly and haphazardly. *The assumption that learning results develop in conjunction with chemical results is unwarranted.*

2.6 The equation of chemical results with learning results

A historical hypothesis concerning the origin of the cookbook problem

The curriculum has been moulded as much by tradition as by rational considerations. Many faculty members teach in approximately the same fashion as they themselves have been instructed. Where does this way of teaching come from? If the teaching of laboratory techniques is considered to be the most important objective, why then situate these techniques in the context of the synthesis of a product instead of training them separately? I have developed a historical hypothesis to explain the existence and persistence of cookbook procedures in chemistry laboratory courses. I admit that it lacks support from the literature on the history of chemistry: I do not know of any historical study on the origin of prescriptions from an educational point of view.

The first institutional chemistry laboratory courses originated in Scotland and Germany in the first decades of the 19th century (Brock, 1992; Ihde, 1984). In those days, chemistry was a young profession, and the frontiers of research could be reached quickly. In the 1820s, Justus von Liebig, the German chemist, was engaged in the analysis of organic compounds. He was in constant need of highly skilled research assistants. He therefore set up a school in which he taught the practical aspects of qualitative and quantitative analysis. His students were working on new analysis problems under his supervision, using his procedures and prescriptions. In this way, they learned research by doing it. From Liebig's point of view, it made sense to equate the chemical results of the work of the students with learning results: they could only obtain results if they had learned to experiment. The chemistry used in education was valid from the professional point of view, and that was what mattered.

However, chemistry quickly developed into a complex profession. A research chemist needed to be acquainted with many more techniques and theories. Since Liebig's instructional strategy had proved to be successful, there was no incentive to question the use of prescriptions in instruction. Gradually, instruction and research separated, because training took more and more time. This constrained the prescriptions: since they were not immediately employed in the context of research problems, the experiments could no longer be open but had to focus on a problem to which the answer was already known. Otherwise, students would not know whether they had mastered the technique. When instructional laboratories developed further, the teacher and the researcher no longer were the same person. This constrained the prescriptions even more, since teachers without research experience in the associated area are less able to judge whatever happens during the execution of the prescriptions. Consequently, the prescriptions had to be written in such a way that students would not make mistakes. Also, the experiments should not lead to ambiguous situations, which neither the teacher nor the student could judge. This urged the writers to add extra details not present in the prescriptions as they originally appeared in research journals, and to select prescriptions with particularly reproducible results.

Throughout the historical development of lab courses, chemical results have been equated with learning results. *The chemical result has been the norm.* Every action, reaction, purification, etc. is justified from the chemical point of view: does it contribute to the result? This equation seemed to promote learning quite well, but this was just a coincidence and is becoming increasingly problematic. Chemistry, as a cumulative discipline, has expanded both in depth and in breadth. Universities attempt to enable students to reach the frontiers of science in just a couple of years. To achieve this, a few experiments have to illustrate all the complicated apparatus, reactions and substances in current use in the various areas of chemistry, within a severe time constraint. If students still are to obtain good chemical results, there is no alternative to giving them excellent prescriptions on how to reach these results. However, this leads to activities that have little to do with current chemical research (Verdonk, 1992).

Prescription experiments are answers to questions of the past. Although education still uses labels like 'organic chemistry', 'physical chemistry', 'inorganic chemistry', research groups nowadays have different names, representing the amalgamation and diversification of the topics: 'heterogeneous catalysis'; 'solid state electrochemistry'. Can students learn to contribute to science when they are only confronted with solutions to old questions?

Selecting prescriptions to combine learning objectives

Not only the cookbook character of each specific experiment is problematic, the selection of such experiments themselves is becoming more difficult too. Chemistry expands, creating ever more facts, techniques, reactions and substances waiting to receive an illustration, preferably in less time with less experiments.

Books on experiments contain many experiments. Each curriculum has to make a selection. But which criteria should be used for this selection? Explicit criteria in books and student guide indicate that the selection should be representative from a chemical viewpoint. However, this implicitly suggests that the selection is not based on learning criteria. This makes it difficult to put experiments into any order: should nucleophilic substitution be treated before or after oxidation? It seems obvious to treat normal distillation before vacuum distillation, because the latter implies more manipulation. In a realistic situation, though, the desired purity may be obtained with more ease in a vacuum distillation than in a normal distillation. *Questions concerning the complexity of topics and their consequent position in the curriculum can only be answered if it is known for what purpose a technique or a theory will be used.* When the purpose of teaching nucleophilic substitution is unclear, how then to specify the sequence and the degree of complexity?

The aspirin experiment is chosen because its techniques are considered to be basic. Another reason is the link with society that aspirin symbolizes. However, other possible criteria such as choosing representative substances or important mechanisms, are not applied. Consequently, the presence of the specific reactions and substances is a random result. This is also true of the other experiments in M&M1. It seems unlikely that an arrangement of experiments based on increasing complexity of manipulation will at the same time provide a structure of increasing complexity with respect to, say, mechanism, or reaction conditions.

Assessment

The use of prescriptions also causes an assessment problem. The goal of assessment is to provide teacher and student with valid information about chemistry learning. When a student carries out a prescription experiment, the results, such as yield and purity, are of a chemical nature. These parameters can be used to assess the quality of the process, but, since the student did not devise the process, can they also be used to assess the student? In some respects, yes: the student shows her or his ability to manipulate the instruments and the glassware (the basic skills) according to the purpose of the prescription. However, in most educational prescriptions, the information is processed in such a way that problems and mistakes are minimized. Consequently, for the better part, the achievement should be credited to the textbook or the instructor. And, many important aspects of experimenting are not assessed at all, because they do not occur in a prescribed experiment.

Of course, most teachers do not judge students only with parameters like yield and purity; they, according to the student guide, should also use the criteria "knowledge, planning, execution, safety, reporting". But such criteria are not specified and left to personal and implicit judgment. Sure, some students perform the experiment quicker, make fewer mistakes, show more understanding, or can formulate their activities and results more comprehensively than others. But again, *assessment will be based on how students learn to carry out experiments, not on how they learn to experiment.*

Another important element in assessing often is the quality of the lab report written by the student. This is also important in the aspirin experiment of M&M1. Such a report also does not describe a student's learning process with respect to experimenting. The student reproduces elements of theory and knowledge (which are not developed by the student), describes the practical procedure (which mirrors the prescription), and gives the actual data. When the experiment was successful the report will not contain anything interesting, and ideally, each student would write exactly the same report.

In prescribed experiments, the chemical results are carefully planned and organized, but the learning results are not, nor is the learning process. In my opinion, it is necessary to rethink the curriculum; to develop new criteria for constructing educational material that explicitly teaches students to experiment; and to develop criteria for assessing student performance concerning this objective. In the next section, I will analyse some solution of these problems.

2.7 Existing solutions to the cookbook problem

The Utrecht curriculum is not all an exception: most textbooks and laboratory manuals show the same characteristics, as do other curricula in The Netherlands (De Jager, 1985) and, as far as I can judge, all over the world. Many other curricula presumably share the same cookbook-like problems, since many scholars have already proposed solutions to the cookbook problem. In this section, I will deal with the solutions that originate from chemistry instructors.

Change is unnecessary

The first strategy is simply to deny that there is a problem. All contemporary chemists have been educated with lecture courses and cookbook-like laboratory courses. A standard reaction to the complaints about the curriculum is: 'Well, we ourselves have learned it this way. It can't be so bad!' Chemists "expect that if students work hard at doing the standard lab work and assignments the activities will somehow bring about understanding" (Trumbull & Kerr, 1993).

There is some truth in this. Learning does not entirely depend upon instruction. The student also has a responsibility. He or she should work hard, ask questions, and prepare for lectures and lab, regardless of the quality of instruction. However, according to this strategy, the responsibility for the learning result is shifted to the student. Any flaw in the curriculum can be brushed aside in this way. To me, learning results should be related to teaching in a clear and explicit way. Another drawback of this non-strategy is that it completely disregards the reasons why students drop out. Some students drop out because they are not smart enough, but many are not intellectually challenged, complain about the quality of instruction, and change to another field. Moreover, diligent, disciplined students not always turn out to be great chemists.

Chemistry instructors often agree that cookbook experiments do not contribute much to learning research. This, however, is not always felt as a disadvantage. Students, they say, should learn the basic skills and techniques first, before they can engage in research-like activities. The snag is whether transfer is possible from this kind of learning to the intended context. It is highly questionable whether breaking up a meaningful activity, like experimenting, into parts, and training the parts separately, will have success. It depends upon the capability of the students to integrate these parts somewhere in the future. It leaves the responsibility for this integration to the student.

For an educational researcher, this position is the hardest to challenge. It is based on *opinions* about quality, not on empirically validated observations. From this viewpoint, research into the quality of education is not necessary, either. Good students will become good chemists, anyway. Nevertheless, I think it would be good if instruction would contribute somewhat to learning.

Adding theory

The real cookbook lab, in which students just follow a recipe without any attention to reasons for doing things, is probably a rare phenomenon. Most lab manuals contain sections on theoretical aspects, such as reaction equations and mechanisms. This information is used in questions which students have to answer. For example, the book or the instructor can ask why sulfuric acid is used in the aspirin synthesis, why an access amount of acetic anhydride is used, etc. This strategy is applied widely in the Utrecht lab course.

The advantage of adding theory is that it makes explicit that prescriptions have a rational basis. However, the student is not challenged to construct justifications or explanations, but has to reproduce established facts. The situation resembles a test instead of a scientist interpreting data. Moreover, this strategy does not influence the laboratory actions themselves. Whether a student knows the correct answers or not, sulfuric acid has to be used. Mulder (Mulder & Verdonk, 1984) showed that students think this questioning is artificial and superfluous; they do not see the point of wasting time on matters that have been settled already: "It *says* that I should use sulfuric acid. If it didn't work, it wouldn't say so!" In research, on the other hand, theoretical argumentations are given to decide upon experiments; experiments are conducted to decide upon theoretical explanations.

Putting blanks into the prescriptions

When students do not need to think in order to execute a recipe, one can make them think by substituting parts of the prescriptions for blank spaces. For example, the aspirin recipe could contain the line 'use .... as a catalyst', or 'add .... grams of salicylic acid', or 'determine which of these products is formed'. This strategy turns lab into a puzzle (Pickering, 1991), but does not change it into a research-like activity. Students are not supposed to find the answers through experimenting but through a priori argumentation based on knowledge of rules and facts. Many blanks can only be filled by students if they look things up in a textbook, since the chemistry is much too complicated to be predicted. Other favourite questions require calculation; in many cases these turn out to be straightforward stoichiometric calculations. However, for empirical reasons, prescriptions often prescribe different ratios, reaction temperatures or voltages then theoretical calculation would suggest (Elzenga, 1991). In the example of aspirin, how could a student know that the optimum result is reached with a twofold excess of acetic anhydride?

Let students select prescriptions from literature

If students have to select a prescription to make a given substance from a number of possibilities, they have to compare in order to reach a reasoned decision (Potter & McGrath, 1989). This makes them think. However, a sensible analysis and comparison of prescriptions can be made only by those who have enough experience with the methods and techniques that are mentioned, which is exactly what students have to learn. Also, comparisons can be made from a variety of viewpoints, such as safety, speed, cost, beauty, yield, purity, and many more, which makes it difficult to agree on which is 'best'. The best criterion perhaps would be to select the procedure from which the student expects to learn the most; instead, students will opt for what they think will be the easiest procedure. Another problem is that TA's seldom have enough experience themselves to judge and supervise each procedure. They frequently have to rely on the rationales provided by teacher's manuals, pushing students into their preferred direction. When a student would propose an unknown method, it will be difficult to judge whether it is feasible or not. Finally, when a method has been selected, the rest of the experiment still is an execution of prescriptions.

Science and society

Why do students make aspirin, and not another white crystalline compound? Because aspirin is a well-known substance in society. Students can derive additional motivation from this, and, it is thought, they develop a better insight on the relations between chemistry and society. Motivational factors indeed are important, and yes, pain relievers are related to chemistry. However, in the laboratory course, the relation between aspirin and society is not so clear at all. Context often is a pretext. It is a wrapping that should be removed quickly to reveal the chemistry of esterification and the techniques of filtration and crystallization; the things the experiment really is about. The aspirin that is made will not be used, but is thrown away as chemical waste, just like any other white powder. Additional texts on aspirin and pain relieving make good reading, but wrongly suggest that chemists know how to relate head aches to chemistry. The molecular representation of aspirin reveals some of its physical and chemical properties, but not the important physiological properties. A professional chemist may have great knowledge of substances and reactions under strictly controlled laboratory conditions, but it is seldom possible to apply this knowledge directly to questions important to society. It takes more than organic chemistry to explain why aspirin is a pain killer. Again, the cookbook character of the experiments themselves is not changed by links with society.

Participation in research

An obvious thing to do to make the lab course more research-like is to have students participate directly in research. This 'research as education' has several advocates (Doyle, 1984; Habraken, 1989; Kirk & Hanne, 1991). The strategy is of course widely employed in graduate programs but is an exception in first year programs. The reasons for this are straightforward. When students should take part in research right from the start, they need almost permanent supervision. In the past, men like Liebig and Van 't Hoff were perhaps able to provide this kind of supervision. Nowadays, students outnumber staff by far. Another problem is that the frontiers of science have progressed considerably since the 19th century. How can a secondary school graduate contribute to modern research in any other way then by performing simple tasks that have to be assigned and thoroughly prescribed? It will take a long time before a student is able to pose a research question, let alone to develop a procedure and obtain results that can be published. Moreover, instruction remains ad hoc from a learning point of view, since the activities in research–and consequently in this kind of education–are chosen for chemical reasons only. It is unlikely that a sufficient coverage of chemistry can be achieved through highly specific research problems. Research often implies endless repetition of the same activities. It is questionable whether learning in such an environment is efficient. The positive point in this approach is that the teacher and the researcher are the same person. Developments in research can thus be transmitted immediately to education, without the time delay that is characteristic of conventional curricula. Participation in research also can be a valuable personal experience for the student, because it illustrates the disappointments, successes and the hard work characteristic of scientific work. But I doubt its value as a learning strategy.

Discovery learning

The first wave of curriculum reform informed and driven by educational research took place in 1960s. It led, among other things, to the idea of modelling laboratory work after science. This led to 'discovery learning'. Unfortunately, a model of science was chosen which proved far from valid. Discovery learning implies an inductivist and positivistic view of science, and suggests that science starts with neutral observation of objective data. Philosophers of science have abandoned this view (Arbib & Hesse, 1986; Chalmers, 1976; De Regt, 1993), and discovery learning has never been an educational success story. To enable students to make the 'right' discoveries, the stage has to be set in a way that is a parody to research. The problem is that discovery learning aims at having students rediscover science, whereas there is no algorithm at all for making a scientific discovery. This strategy has already been adequately criticized elsewhere (Hodson, 1985; Kirschner, 1991).

Differentiating between a learning phase and an application phase

In the laboratory, students are confronted with many things that are knew to them. If one takes the viewpoint that a complex whole is made up of parts, it is sensible to train these parts separately. Johnstone (Johnstone & Letton, 1990; Johnstone & Wham, 1982) suggests that the cookbook problem arises from the fact that students in the lab are overwhelmed by so many new experiences. Their working memory is overloaded, and they stop thinking altogether. He therefore suggests to divide laboratory instruction into two cycles. First, students receive training in laboratory techniques using prescriptions that are as clear as possible. Second, the students have to apply their knowledge to solve a problem in an analogous situation. An example would be to first train the titration of acids with bases using stock solutions of acetic acid and sodium hydroxide, and then have students analyze the concentration of acetic acid in vinegar.

Such a strategy probably is very efficient for training skills and routines, in which there is a standard procedure or algorithm for a standard problem. Thus, this strategy optimizes the skills part of chemistry, but not the research part. I cannot believe that this strategy can lead to the desired learning results with respect to experimenting, since, in more open situations, the real difficulty is not the correct application of techniques, but the recognition of the analogy present. In the titration of vinegar, students not only have to perform a correct titration, they also have to take a suitable sample and dilute the acid to the concentration range of the base. This problem is not analogous, it is new. The problem of taking a sample can be trained separately of course, but that would lead to an infinite regress of sub-problems within sub-problems, which quickly lose their meaning.

Goedhart (Goedhart, 1990) reports on his attempt to teach spectrophotometry in this way. He observed and described that, in the application cycle, the students very often pursued completely different and unexpected strategies. They did not see the analogy. Consequently, they were unable to solve the problem he gave them.

2.8 Conclusion

I conclude that the cookbook problem so far has not been solved. Most approaches still rely on prescriptions. Some strategies, like adding theory, make students think, but in most cases this thinking has no direct consequences for the lab work itself. Other strategies, like research as education, rely on processes that remain fully implicit and ad hoc. Or, like discovery learning and the application cycle, they are based on a naive, algorithmic view of science. A suitable framework for investigating how students come to an understanding of organic synthesis is still lacking. In the next chapter, I therefore take one step back from the laboratory, to reflect on the problem of understanding itself. If understanding is a prerequisite for experimenting, and I think it is, what exactly is meant with 'understanding'?

3 A hermeneutic framework

3.1 Knowledge versus understanding

The major objective of my study is to determine the relations between teaching and learning in organic synthesis. The teaching goal is to prepare students for doing research in this area. I can only investigate my question if the learning results are related to teaching, and if teaching prepares students for research.
In the previous chapter, I discovered that current teaching is not consistent with respect to this goal. Although 'learning to experiment' is an important objective in name, the realized curriculum is more adequately described in terms of learning facts and learning laboratory techniques. Students achieve learning results in these respects: they are able to pass the paper and pencil examinations and to carry out the prescribed laboratory experiments successfully. However, a complaint uttered widely in literature is that students, following cookbook experiments, do not acquire understanding. This was confirmed by my case study on the aspirin synthesis experiment. Students are, broadly speaking, unable to justify the choices made in this procedure; they do not even realize that choices are continuously being made. I found that it was not necessary for them to understand, to carry out that experiment. For that reason, I doubted whether such teaching contributes to the desired goal of learning to do research.
If teaching does not aim at preparing students for research, then the learning results in this area are not related to teaching. If understanding is necessary for experimenting and for doing research, and if current teaching does not contribute clearly to this, it seems that I should focus further on understanding. In this chapter I therefore reflect fundamentally on the problem that students in cookbook experiments do not seem to understand, although they clearly know a lot of things. My aim is to clarify understanding as such, proceed to understanding in relation to chemical research, and end with understanding as a learning result in an educational situation. From this analysis, I hope I will be able to provide the desired teaching structure.

Up till now, the word 'understanding' has been used in a rather loose sense. I have been associating it with the rationale of laboratory activities and with linking 'theoretical' knowledge to 'practical' decisions. What exactly is understanding?
To start this elaboration, I suggest to distinguish understanding from the kind of thing that *is* achieved by the curriculum. Understanding is the quality lacking in students who are otherwise able to perform well in cookbook experiments and tests. I acknowledge that students *know* a lot of facts, formulae, theories, and procedures. They know, for instance, how to carry out a Büchner funnel filtration. In this respect, the often used distinction between knowledge and skills does not help. Whatever can be recorded and communicated in some material format–data, procedures, models, theories, prescriptions–can be called *knowledge*. Thus, McMurry's Organic Chemistry is knowledge. So is Vogel's manual of synthesis procedures.
What about understanding? Is understanding something that is external to knowledge but that can be attached to it, for example through explanation? Or it is essential to knowledge and thus cannot be separated or attached without changes in meaning? This implies that the word 'knowledge' has at least two meanings. If understanding is external, it is

possible, to 'know' without understanding. This can be little more than the ability to reproduce. This kind of knowledge could perhaps better be called *information*, to distinguish it from knowledge that is understood. From this point of view, students in cookbook experiments merely possess information.

A first clue to investigate the character of understanding is to compare the way knowledge is achieved through research and through education. In research, an object of research is chosen, investigative procedures are carried out, and knowledge of the object of research results. In education, the direction quite often is reversed. Facts and theories (information) are communicated to students in the form of rational reconstructions and students are to understand these as knowledge. Experiments are programmed to prove the correctness of hypotheses; to demonstrate how to carry out procedures that turned out to be successful in research; and to teach students how to handle the equipment. These experiments are not meant to establish new knowledge. The question is: can these processes lead to the same results? Can the knowledge of chemical researchers have the same fundamental character as the knowledge of students? What is the nature of 'understanding' in these processes?

Logic suggests that this reversal is legitimate if there is a correspondence between knowledge and the object of research. If this is the case, it is at least logically possible to start with teaching knowledge, and end with students understanding this knowledge in the same way as the researchers. I will investigate this position in the following section.

3.2 Objectivism

Facts can be given in the form of propositions. "The electronic structure of carbon in its ground state is $1s^2 2s^2 2p^2$"; "The formula of water is H_2O"; "When water is added to the reaction mixture, aspirin precipitates". Such statements can be communicated directly to students if understanding is seen to be external. Whether the first proposition is understood or not does not change the fact that carbon has a ground state which has a certain electronic structure. This fact can be taught and learned. The proposition can be seen as an answer to a question: "What is the structure of the carbon atom in its ground state?" For anyone posing such a question, the answer (obtained through research or through literature) will be meaningful. The caveat is that students normally do not pose such questions. They do not even know what would be a meaningful question in these areas alien to them. Still, they receive the answers, in the form of propositions, and they have to make sense of them. If students ask why they have to know this, the typical answer is: "That's how it is".

Central in this framework is the assumption that objects like the carbon atom exist in the real world, independent of human beings, and that their properties can be described correctly and objectively. The philosophical position that lets knowledge claims correspond in some way with things in the world is often called *realism*. The nature of the correspondence is investigated by analytical philosophy. I prefer the term *objectivism* to refer to this framework because this term clearly shows the basic category: the object. The use of the word *object* immediately evokes its counterpart, the *subject*. This distinction goes back to Descartes, who grounded knowledge in the indubitable existence of the reflecting Self: *Cogito, ergo sum*. From the existence of the subject, he could deduce the

existence of the world, and the possibility of acquiring true, that is, objective, knowledge of the world through science. This philosophy highly influenced Western thought. It proved to be extremely versatile in the natural sciences, or, perhaps, it created the possibilities for doing the thing we now call science.
Objectivism can be seen as a specific elaboration of the basic intuition that the world around us is both real and comprehensible. I largely agree with Lakoff's (critical) discussion (Lakoff, 1987), pp. 160-161), in which he describes objectivism as the philosophical position which holds that:

> All of reality consists of entities, which have fixed properties and relations holding among them at any instant. (..) Among the properties that things have, some are essential; that is, they are those properties that make the thing what it is. (..) All the entities that have a given property in common form a category. (..) The entities in the world form objectively existing categories based on their shared objective properties.

The human mind–the subject–represents external reality in a way that resembles a mirror ('the mirror of nature'): entities and categories in the objective world are represented by symbols or concepts (o.c., pp. 163-167):

> Human reason is accurate when it matches objectivist logic, that is, when the symbols used in thought correctly correspond to entities and categories in the world and when the mind reproduces the logical relations that exist objectively among the entities and categories of entities in the world. (..) Knowledge consists in correctly conceptualizing and categorizing things in the world and grasping the objective connections among those things and those categories. (..) Existence and fact are independent of belief, knowledge, perception, modes of understanding, and every other aspect of human cognitive capacities. No true fact can depend upon people's believing it, on their knowledge of it, on their conceptualization of it, or on any other aspect of cognition. (..) Our conceptual system, that is, the symbol systems that we use in thought, are innate and are made meaningful via their capacity to correspond correctly to entities and categories in the world. In other words, our inborn mental representations are 'semantically evaluable', that is, capable of being true or false and of referring correctly to entities and categories in the world. (..) We acquire our concepts, that is, the symbol systems that we use in thought, through accurate sense perceptions in such a way that they correspond systematically to entities and categories in the world. (...) Linguistic expressions get their meaning only via their capacity to correspond, or failure to correspond, to the real world or some possible world; that is, they are capable of referring correctly or of being true or false.

3.3 Influences of objectivism on education

The problem is not that many scientists in fact are objectivists. Objectivism is a legitimate epistemological position. The point is whether objectivism is a suitable framework for science *education*. It seems to me that objectivism is the implicit philosophy used by writers of textbooks and curriculum developers. Many common strategies in education–or perhaps 'instruction' is a more appropriate term–make sense from the point of view of objectivism.

Knowledge, according to objectivism, can be represented in words, in books, in formulae, in pictures and models, and hence can be taught in a process of transfer. Concepts are used to define and categorize related pieces of knowledge. For example, the concept of chemical reaction is used to describe specific processes in which substances change into other substances. Concepts themselves are mental objects (or 'third-world objects', as Popper would call them). A concept is true if it refers to valid relations, processes or principles in the real world. For example, at the moment the concept of conservation of energy/matter is considered to be true, whereas the concept of conservation of heat is not anymore. Since these concepts refer to objective knowledge, introducing students to concepts by way of telling them is an efficient way to teach. Then they know them too. A concept can be known in the same way as the fact that the earth is round can be known. In fact, understanding has no role to play in this framework. Understanding a concept is the same as knowing the concept. It simply means being able to refer correctly to things in the world. Scientists, though, can be mistaken, and render descriptions which, in the long run, prove to be incorrect, like the phlogiston theory. Thus, knowledge always remains fallible, although the ultimate goal is to reach absolute truth. Science progressively replaces old concepts for better ones.

Sometimes, old concepts remain useful in restricted areas, although they are not 'really' true. It is still considered correct when a student uses the word 'force' in a Newtonian sense, although Einstein's rendering is more fundamental. However, other uses of the word 'force' are called *misconceptions*: a correct concept is correct for anyone, anytime, anyplace. It is not a question of opinion. It is the task of science education to inform students on how things really are.

Although scientific concepts are valid regardless of situation, contextual features often obscure a clear view of the object of knowledge. Objectivist instruction therefore has a tendency to isolate and highlight the elements that are considered important. It often focuses on the objects and concepts in abstraction before situating or illustrating them in more realistic situations. A schematic drawing, for example, easily draws attention to relevant features, whereas a photograph can be ambiguous (Bastide, 1990). A picture of a beaker filled with water does not clearly show that water consists of H_2O particles. It is easier to demonstrate a principle of chemical reaction in the laboratory with pure and simple substances than with complicated real life situations like preparing food.

Categorizing and conceptualizing only work if particular entities share 'essential properties'. It is therefore natural to focus especially and sometimes exclusively on such shared features, instead of having to account for a multitude of irrelevant features too. This is one step away from reductionism: explaining similarities with an appeal to deeper, more fundamental entities. In chemistry, the wealth of phenomena can be reduced enormously using concepts like element, valence and bonding. Objectivism legitimizes this kind of reductionism. The phenomena, as we experience them, are the surface. The real, fundamental entities lie underneath and explain everything on the higher level. That is, if there is a correspondence between these fundamental entities and the world.

3.4 Objections against objectivist education

Objectivism consists of *logical* relations. An interesting thing about logic is that it is possible to manipulate logically without understanding. Computers are an example; objectivism transplanted to education provides another example. Objectivism emphasizes knowledge, but does not pay explicit attention to understanding. An objective truth is true, no matter if it is understood or not. The meaning of a proposition simply is its capacity to refer to something in the world. This is purely logical or linguistic meaning, and has little or nothing to do with human understanding of meaning.

Objectivist science education presents, explains, and illustrates this system of logical relations and categories. Experiments are done to introduce new topics, to raise attention to new features of reality to be explained, and to provide illustrations. Scientific research can be characterized by the attempt to find objective relations in the sense of objectivism; objectivist science education presents the results.

Probably it is possible to learn the scientific system in a mindless way, just to be able to reproduce the facts and apply the rules in test situations. I expect nevertheless that many students will also try to make sense of what they learn. When they succeed, they acquire an understanding of the logic of the system. This is a rational reconstruction of the results of research. Since there is a correspondence between reality and the knowledge claims laid down in the system, understanding the system is understanding reality.

This conclusion, however, depends upon the correctness of the correspondence assumption. This assumption is itself object of debate among philosophers of science. The correspondence principle uses reductionism as a tool: complex phenomena are stripped of those features not influencing the phenomenon to be explained. The relevant features are put together in a model representation. It then becomes possible to use the model to predict phenomena. Strong reductionism holds that the model completely covers the phenomena. However, many philosophers of chemistry have argued that strong reductionism cannot be true (Prigogine & Stengers, 1984; Primas, 1981; Van Brakel, 1994; Van der Vet, 1987).

Primas, for example, argues that each reduction is made from a certain viewpoint. "In the physicist's description electrons and nuclei are correlated by Einstein-Podolsky-Rosen correlations so that neither electrons nor nuclei exist as individual objects. In the chemist's description electrons and nuclei are not correlated in the sense of Einstein, Podolsky and Rosen (in spite of their strong electromagnetic interaction), so that nuclei exist as classically describable individual objects" (Primas, 1981), p. 317). Reducing chemistry to physics is accompanied with the loss of concepts such as localized electrons. Physics may be more fundamental but is not necessarily more useful. Certain scientific questions can only be answered on a higher hierarchical level, because it is at these levels that properties considered relevant *emerge*. "The theory of emergence assumes that there are different levels of existence such that entities on a higher level are characterized by specific properties that do not occur on lower levels, and such that it is impossible to deduce the characteristics of a higher level from those of a lower level. (...) There are facts which are not ultimately accounted for by the intrinsic properties of elementary objects. For example, substances may have a temperature, single molecules do not" (o.c., p. 312).

Reduction often is useful, but not for all purposes: "We are free to choose between mutually exclusive viewpoints, but every choice has to be paid for by the loss of complementary knowledge" (p. 351). There is no objective way to choose between viewpoints. It is the reverse: *objectivity is a consequence of viewpoint*: "The question 'do atoms really exist?' is much too naive to allow a clear-cut answer. *If* we interact with matter in a way that emphasizes the space-time structure and its description via the Galilei group, then we have a starting point for a sensible answer. However, a priori there is no reason which would force us to adopt this viewpoint. That is, an elementary particle does not exist as a thing-in-itself but the atomic idea is *enforced* by the adopted viewpoint" (p. 347).

Thus, I assume that reality is underdetermined by scientific models, since it is possible to investigate reality from an infinite number of viewpoints. Understanding the logic of specific models and systems cannot be the same as understanding reality, because this logic does not contain the reflections on choosing a viewpoint. Scientists who do the research *choose* a viewpoint, whereas students are implicitly forced to *take* the same viewpoint. Since this is presented as a logical consequence of the system, it is tacitly suggested that there are no other viewpoints.

Problems occur in several ways. In chapter 2 I already described the cookbook problem in detail. This problem, it seems to me, can be traced back to an unproductive application of objectivist principles in education. But it is also well known that students do not always apply scientifically 'correct' concepts to their daily life contexts. And, they may experience the tension between models used in physics and models used in chemistry (Van Hoeve-Brouwer & De Vos, 1994). I think that these problems cannot be solved within the borders of objectivist philosophy. It does not work to maintain that having objective knowledge is the same as understanding reality, and to maintain that providing students with the logical system of chemistry and adding the skills necessary to use the apparatus, establishes the foundations for future scientists. I would like to challenge the objectivist framework. In the next section, I therefore start to search for an alternative.

3.5 Phenomenology

In the objectivist framework, understanding is external to knowledge. Having knowledge of the right facts, theories and procedures is what matters, understanding these (whatever that may be) is not relevant. But what happens when understanding is seen as an essential characteristic of knowledge? In that case, if students are to understand like scientists do, it seems that, instead of starting with the results, they should start with the phenomena that are investigated and try to understand these in order to be able to construct knowledge. This reflection drew my attention to a philosophical tradition which bears the word 'phenomenon' in its name: phenomenology. In this section, I give a very brief outline of phenomenological thought as far as relevant for my purpose, which is to clarify the concept of understanding. It is largely based on the *Cartesian Meditations* by Edmund Husserl (Husserl, 1950).

Phenomenology can be seen as a reaction against objectivist tendencies. Phenomenologists take another basic intuition as a starting point: We know about the world through experience and consciousness. Consequently, these are more basic than objects.

Phenomenology literally is the study or description of phenomena; and a phenomenon is just anything that appears or presents itself to someone. Husserl denies the existence of a 'real' world of objects if that implies that this world is wholly independent of the 'subject' that experiences this world. According to Husserl, Descartes wrongly characterized the 'I' as a thinking 'thing'. He uncritically accepted a specific idea of science, and hence of what philosophy as a science would have to be like: namely an axiomatic system, modelled upon geometry and the mathematical natural science of that time. If 'I exist' is taken as an axiomatic premise, from which 'the world exists' is to be deduced as a conclusion, then the meaning of the term 'exist' must remain the same throughout; otherwise the argument would not be valid. Thus, the ontological status of the 'I' and of the world would have to be the same. According to Husserl, the status of the I, which he calls the Transcendental Ego, is not comparable: it is through the Ego that the objects in the world gain their status as existing objects which then can be experienced as such. The constituting subject therefore necessarily is not a part of that world. The assumption that objects exist, and that conscious subjects–and their mental states–exist in the same 'objective' way as a part of a natural world, must be dropped. Claims that objects exist and have certain permanent properties are always mediated and constituted by the experiencing subject. In other words, phenomena and consciousness are more fundamental to knowledge than objects. The experiencing subject acquires a strictly personal history: it develops a repertoire of experiences with phenomena, from which objects are constituted. Those objects with which a subject has had experience form a part of the description of the self. Expectations–anticipations, as Husserl calls them–are based on the experiences a particular subject has had. Husserl calls these anticipations 'horizons'. Experience is the basis of the ability to conceptualize and to create ontologies of physical objects. Since these objects always exist as objects of consciousness, the question is not whether what we say about objects is true, but whether it is *meaningful* to describe one's conscious experience in that particular way. True knowledge in the form of complete descriptions of objects in the world is simply impossible to achieve. "One finds that what one means is not that certain experiences, the 'true' ones, correspond to facts in a realm independent of experience, but rather that a judgment is true when it is an element in a set of judgments which together characterize a coherent system of experiences" (Hammond, Howarth, & Keat, 1991).

Knowledge of the natural world thus can be achieved through experience that mediates between the world and consciousness. Knowledge in the forms found in textbooks of science is not the same: this knowledge is not a meaningful description of the conscious experience of the student. I suggest to differentiate between these two kinds of knowledge. The second form is information. The first form, '*meaningful description of conscious experience*', is an explication of *understanding*.

This philosophical position has implications for teaching and learning. If it is true that experiencing phenomena will lead to different conscious states and hence to different knowledge and understanding than the experience of teachers talking about phenomena and objects, then, consequently, education should be careful in deciding when to build knowledge through transfer of information, and when to contribute to the development of a personal history through the presentation of phenomena.

3.6 Hermeneutics

In phenomenology, understanding is a way to order personal conscious experience. Consequently, it seems that *introspection* is the road to knowledge. Husserl has often been criticized for this rather idiosyncratic tendency in his philosophy, which threatens to reduce knowledge and understanding to a private affair instead of being open to public scrutiny. For this reason I turn to an elaboration of phenomenology that shifts the focal point of attention from consciousness to *language*. This necessary development is provided by philosophical hermeneutics, especially as it is elaborated in Hans-Georg Gadamer's 1960 volume *Wahrheit und Methode* (Truth and Method; (Gadamer, 1986).

Gadamer's philosophical hermeneutics pays considerable attention both to language and to understanding. Therefore, it seems a promising philosophical framework. The central elements in hermeneutics–as I see it–are the triad *interpretation-understanding-application*; the idea of *context*; the notion that *language* is the medium in which we live; and the idea that all understanding is *historic*, that is, takes place in a historic process that cannot be objectified.

Hermeneutics as a method

The origin of hermeneutics lies in its use as a *method* for interpreting texts, especially texts that are difficult to understand because written in a different culture or time. Hermeneutics as a method is a unity of interpretation, understanding and application. The aim is to *understand* a text. To achieve this, one has to *interpret* those elements that are not yet understood. In order to determine whether an interpretation is valid, it should be *reapplied* to the text as a whole, to see whether it makes sense, that is, adds to a better understanding of the text. Such an application will reveal new problems or inconsistencies, inviting further interpretation, etc. It is this method that is elaborated by Gadamer into a *philosophy*. Gadamer metaphorically regards the world as a text to be interpreted.

Context

In interpreting a text, the meaning of a word depends on the other words in the sentence, the *context*. Likewise, the meaning of a sentence depends on the surrounding sentences. Philosophical hermeneutics metaphorically regards the world as a text: the meaning of the things in the world depends on the context, on the specific constellation in which we experience things in the world. *Without* a context, things are meaningless, like an unknown word without a sentence. A *different* context implies a different meaning. Thus, knowledge claims have a meaning, and this meaning depends on the context. This is clearly different from objectivist ideas, from which point of view knowledge claims are either true or not true. This does not depend upon context but on facts of the matter. For example, water is H_2O in each and any context.

The difference in attitude can be illustrated with Polanyi's criticism of the objectivist ideal: "The paradigm of a conception of science pursuing the ideal of absolute detachment by representing the world in terms of its exactly determined particulars was formulated by Laplace. An intelligence which knew at one moment of time–wrote Laplace–'all the forces by which nature is animated and the respective positions of the entities which compose it (...) would embrace in the same formula the movements of the largest bodies in the universe and those of the lightest atom: nothing would be uncertain for it, and the future, like the past, would be present to its eyes'. This ideal of universal knowledge is mistaken, since it substitutes for the subjects in which we are interested a set of data which tell us nothing that we want to know" (Polanyi, 1962). What we want to have is not perfect, absolute knowledge of the movements of molecules, but what this stands for: a hole in the ozone layer, a pain-killing drug, etc. Meaning is related to our interests, and interests are highly influenced by contextual features.

The meaning of knowledge thus does not come from the things in themselves, but from the context in which things are experienced. *A context is a whole of entities that give meaning to each other*, in the widest sense.

Language

The context of an entity is not always articulated in language. Things exist in the world, and world is not words. Or is it? If knowledge of things in the world should be more than a personal conviction, *consensus* should be reached. This implies finding the words to describe the experience, the context, and the point of view. Like phenomenology, Gadamer denounces the Cartesian subject-object distinction and stresses the importance of experience. But unlike Husserl, Gadamer does not focus on consciousness but instead focuses on the medium of understanding, which to him is *language*. In this way he avoids getting tangled with speculations about cognition. For Gadamer, reality exists only within language: "Being that can be understood is language" (Gadamer, 1986), p. 478)[1]. In this way the metaphor of the world as a text is taken almost literally: the context is seen to exist only in language. This should not be taken to mean that material objects are not made of matter. The point Gadamer wants to make is that in as far as we understand the world outside us, we do this with language. In as far as we are unable to reflect on our actions and sense perceptions in the light of conscious intentions we are part of that world, and the distinction between the acting and interpreting subject and an outside world is meaningless. Although a reflection may be immature and tentative, it is always in language, if not to describe the intention or experience itself, then at least to say 'something' about it. A child who still is oblivious of itself as an individual cannot interpret its actions in terms of meaningful behavior. It does not yet live in language. So do anthropologists venturing into alien cultures: they do not see what is going on until they find the words and concepts to describe their experiences. Before that happens, things are meaningless to them, and they move around like children in a science lab.

Whoever uses concepts like 'reality' uses a language. Thus, language is the fundamental characteristic of being, and things can be seen to 'exist' in language only. In this respect, Gadamer follows Heidegger rather than Husserl: "Discourse is the Articulation of intelligibility. Therefore it underlies both interpretation and assertion. That which can be Articulated in interpretation, and thus even more primordialy in discourse, is what we have called 'meaning'. That which gets articulated as such in discursive Articulation, we call the 'totality-of-significations'. (...) The intelligibility of Being-in-the-world–an intelligibility which goes with a state-of-mind–*expresses itself as discourse*. The totality-of-significations of intelligibility is *put into words*. To significations, words accrue" (Heidegger, 1962), p. 203[2]). A context thus has the characteristics of being articulated, being meaningful, and being a totality: an articulated, meaningful totality.

Fusion of horizons

How does interpretation and understanding occur in unknown non-verbal contexts? Interpretation always is interpretation of something. This something, which Gadamer calls *Sache*, is not necessarily a material object. A *Sache* is the meaningful *issue* around which conscious experience crystallizes. Babies learn to discriminate persons from the totality of their sense impressions. Astronomists learn to discriminate background radiation from

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[1] My translation of "Sein, das verstanden werden kann, ist Sprache". I was not entirely satisfied with Barden & Cumming's translation (Gadamer, 1975), so I choose to translate citations from Wahrheit und Methode myself.

[2] The German text has: "Rede ist die Artikulation der Verständlichkeit. Sie liegt daher der Auslegung und Aussage schon zugrunde. Das in der Auslegung, ursprünglicher mithin schon in der Rede Artikulierbare nannten wir den Sinn. Das in der redenden Artikulation Gegliederte als solches nennen wir das Bedeutungsganze. (...) Die befindliche Verständlichkeit des In-der-Welt-seins *spricht sich als Rede aus*. Das Bedeutungsganze der Verständlichkeit *kommt zu Wort*. Den Bedeutungen wachsen Worte zu" (Heidegger, 1986).

instrumental errors. Sociologists 'see' power in human relations. An issue is always experienced within a context and from a point of view. Gadamer expands the metaphor of viewpoint towards the notion of 'horizon'. Interpreting is like moving through a landscape. From each viewpoint, the issue is different, is seen from a different angle, against a different horizon, or not seen at all. But these horizons can 'fuse', when someone understands that different interpretations both are illuminating ways to talk about the same thing. Likewise, people can understand each other through communication in a process of fusion of horizons: they move to each others viewpoint. This is a process in language. Language enables us to engage in dialogue and interpret and understand the issue as it is seen from the point of view of the other. Knowledge is the fixation in language of a *consensus* between those involved in the discursive process on how to interpret an issue in its context. Knowledge is a result of understanding and as such is more than information.

This process is comparable with the transformation that takes place in science from interpretation to knowledge, and from hypothesis to fact. As long as the interpretation is tentative, statements are full of modifiers: "I think that ....", "Under these circumstances ....", leaving room for challenge: "But you might as well say ...". According to Latour, "by being sufficiently convincing, people will stop raising objections altogether, and the statement will move toward a fact-like status" (Latour & Woolgar, 1986), p. 241). "At the frontier of science, statements are constantly manifesting a double potential: they are either accounted for in terms of local causes (subjectivity or artefact) or are referred to as a thing 'out there' (objectivity and fact). (...) It is because the controversy settles, that a statement splits into an entity and a statement about an entity" (o.c., p. 180). Controversies are not settled because the hypothetical entities suddenly show up for everyone to see: molecules can only be 'seen' using the kind of equipment that finally convinced scientists that molecules exist. The third edition of Peter Atkins' widely used textbook Physical Chemistry (Atkins, 1987) starts with the sentence "We know that atoms and molecules exist because we can see them". This statement is followed by a 'field-ionization spectroscopy' photograph, showing an orderly pattern of black dots with concentric rings representing 'a platinum tip of about 150 nm radius'. The sentence is dropped in later editions, presumably because the student-readers do not 'see' the atoms or molecules in the picture.

One cannot check the truth of statements like 'The molecular formula of water is H_2O' without using a network of laboratory activities which mutually define each other, that is, without taking the point of view from which an issue is experienced as having a molecular formula. The matter is not if molecules 'really' exist or not, but that, given a point of view, certain interpretations make sense whereas others do not. General consensus on interpretation means that a new fact comes into existence. The character of this fact depends upon the character of the viewpoint. Adopting a viewpoint is something you have to do yourself; it is of no help when someone else–a teacher–tells you how things look like when you would adopt his or her standpoint. It is as if someone is describing a non-figurative painting to you in terms of the emotions evoked by it.

Gadamer has argued that the language chosen to describe experiences–and to construct facts in science–is not at all arbitrary. Every question already anticipates an answer, and thus shows the beginning of an understanding. Although in scientific research the questions are mediated by the possibilities of material manipulation, they still are constituted by language, which enables understanding and consensus. A scientific result is meaningful only if it can be seen as an answer to a question. If not, interpretation and understanding are not possible. Gadamer maintains that the interpretive problem cannot be resolved by simply inventing strings of technical terms. Interpretation is the right understanding of the issue itself, which occurs in language as a medium. "Words are, in a mysterious way, bound to what is represented; they have a right to belong to the Being of what is represented" (Gadamer, 1986), p. 420[1]). That is why the discovery of a suitable word often comes as a revelation.

Interpretation-understanding-application

According to Gadamer, the hermeneutic phenomenon is to see the world in a unity of interpretation, understanding, and application. Speaking of 'viewpoints' implicitly suggests detached observation. But this is taking the metaphor too literally. Interpretation is not reproduction of reality before the eyes, it is always also an application. We are part of the context in that we play an active role in constituting the object. We interpret the world we encounter by applying our own preconceptions and prejugments. We test our existing conceptual framework. Understanding is the resulting coming into being of meaning. This appears to us as a consequence of an interpretive effort. But in a way understanding is also prior to interpretation: interpretation already presupposes a meaningful totality.

We do not understand a *Sache* unless we can see it in its context, and know how to apply our understanding when we move through this context: "Understanding appears to be an aspect of application and knows itself to be so" (o. c., p. 346[2]). The nature of the *Sache* becomes clear in this process.

The historic character of understanding

According to Husserl, understanding is the meaningful ordering of conscious experience. Knowledge is not an experience, hence it makes sense to differentiate between knowledge and understanding. What is the character of understanding in hermeneutics? What is the difference with knowledge, or could one just as well use the triad interpretation-*knowledge*-application?

The concept of understanding is difficult to explicate. Somehow it evades analysis, although it is often used matter-of-factly. For instance, tests and examinations are often explicitly meant to assess students' understanding. But correct answers to test questions are not always proof of understanding: students can reproduce facts without knowing what they mean. Consequently, teachers often characterize students not only by referring to their mark, but also by referring to the amount of display of understanding. This can be: asking a good question; giving an unexpected but thoughtful answer; or a planning of activities that reveals an interesting purpose. Seldom is understanding equated with 'the student did exactly what he or she was supposed to do'.

On the other hand, scientific laws, concepts, objects, etc., are not formulated in terms of understanding. What is the understanding in the statement 'acids can donate a proton'? Such a statement can be uttered by a pupil who learned it by heart to reproduce it on an examination, but certainly Brønsted and Lowry must have had more in mind. They laid

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[1] "Dem Wort kommt auf eine rätselhafte Weise Gebundenheit an das 'Abgebildete', Zugehörigkeit zum Sein des Abgebildeten zu".

[2] "Das Verstehen erweist sich als eine Weise von Wirkung und weiß sich als eine solche Wirkung".

down their understanding in a statement, but the statement itself does not include their understanding anymore. This is the clue to what Gadamer calls the *historic* character of understanding. In hermeneutics, understanding is a process that exists in time only. It is a thoroughly *historic* concept.

The goal of (natural) science is to create *objective* knowledge. From the point of view of hermeneutics, the fundamental character of such knowledge is not that it correctly refers to how things really are. The crucial element is that it is a-historic. Scientific objects and processes are lifted out of time: they are exactly the same here and now and at any other time and place. Only then is it possible to speak of '*the* reaction of ethanol with acetic acid'; 'water is H_2O', '$\Delta G = \Delta H - T\Delta S$'. There is no need to refer to a specific occasion in which these statements happen to be the case. In this form, science is able to *predict and control*. I can predict with absolute certainty that, if I were to put together salicylic acid, acetic anhydride and sulfuric acid, then I would produce aspirin. For this, I only need to have the pure substances and clean beakers: laboratory conditions. The success of an experiment is determined by its repeatability, that is, the repression of all contingent factors. The ideal of objective knowledge is to be exhaustive, to capture every aspect of the object and process. This may not always be possible in practice, but it is a thinkable ideal. The concrete liquid substance called water cannot be defined completely, but if water is seen as H_2O it can be made objective. The properties of a molecule do not depend on history: a molecule has no history. It does not exist in *our* time.

Objective conditions do not exist outside the laboratory. In nature and in daily life, processes never repeat themselves in a timeless fashion. Even in the laboratory, the history of substances can be relevant: impurities left after a synthesis procedure can have enormous effects on various properties. But ideally, such effects are either absent or completely controlled.

However, science also has a necessary contingent aspect: the experimenters themselves cannot escape time. From the point of view of the scientist, nothing is ever the same. You cannot lift yourself out of life and history to give an objective account of experience. There is always a relation between object and subject. But in order to be truly objective, precisely this relation has to be denied. Husserl already stressed this point. Implicit in the concrete experience of an object is the anticipation that the object can also be experienced under different conditions, in different ways. The *reality* of an object experienced in real life consists precisely in its having *un*experienced and *un*exhausted aspects. There is no way to exhaust this experience and reach objectivity. The objectivity of scientific objects and processes on the other hand consists in precisely defined properties. "[Husserl's analysis] showed that the concept of objectivity of the sciences is an exception. Science is anything but a fact that could be taken as a starting point. On the contrary, the constitution of the scientific world poses a peculiar problem, that is, to clarify the idealization that comes with the sciences" (o.c., p. 263[1]).

In this respect, phenomenology and hermeneutics are diametrically opposed to objectivism. In objectivism, the phenomena are appearances, whereas the thing-in-itself is real. In phenomenology, the phenomena are real, whereas the thing-in-itself is a construct.

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[1] "[Husserl's Analyse] ließ den Objektivitätsbegriff der Wissenschaft als einen Sonderfall erscheinen. Die Wissenschaft ist alles andere als ein Faktum, von dem auszugehen wäre. Die Konstitution der wissenschaftliche Welt stellt vielmehr eine eigene Aufgabe dar, die Aufgabe nämlich, die Idealisierung, die mit der Wissenschaft gegeben ist, aufzuklären".

Gadamer elaborates this point further to show that the life-world in this respect is opposed to the objective world of the sciences: "The concept of the life-world is opposed to all objectivism. It is a truly historic concept; it does not indicate a universe of entities. The infinite concept of a true, objective world cannot be generated meaningfully as a historic experience from the infinite progression of historic human worlds" (p. 251[1]). Statements, interpretations, scientific facts, are the results of reflective thinking: conscious thinking reflecting the projection of experience on consciousness. This thinking process itself is part of life and history and cannot be objectified. The knowing subject and the object of knowing are related in a historic process of understanding. This *is* understanding: knowing that at this moment, in this situation, this is the right thing to do, the right thing to say, the right thing to see. It is only the *results* of understanding that can be separated from life, and that can be made objective, if that is what is wanted. "*Understanding is (...) the original mode of Being*, the Being-in-the-World. Understanding is what constitutes what it is to be in the world, before all differentiation of understanding into the various ways of pragmatic or theoretical interest sets in" (p. 264[2]).

Understanding is a subjective experience belonging to time and context. To objectify understanding is trying the impossible: there is no viewpoint out of time and context. "Objectifying consciousness, although it strains its mind to penetrate the laws of the appearances, can in fact never really know what is alive" (p. 257[3]).

It would thus be a mistake to identify understanding with the possession of objective knowledge. Understanding is an experience, a process. There is no need to repeat this experience in the way science repeats its experiments. It has an unmediated certainty that does not depend on controlled verification. That would be impossible, too, for every subsequent experience will be seen in the light of previous understanding. "Completed understanding constitutes a state of new freedom of the mind. It implies the versatile potential for explaining, seeing relationships, drawing consequences, etc." (p. 265[4]).

It is this phenomenon that I will try to investigate. *If educators complain about students who do not understand, I take this to mean that the students missed the historic experience that would have allowed them to interpret an issue as an object of science.*

Objections against hermeneutics

In a previous section, I have criticized the objectivist framework. However, from the objectivist point of view, hermeneutics has its problems too. A first problem is that the idea of things deriving their meaning from a context seems to lead to a holistic impasse. When everything depends upon everything else for its meaning, how is it possible to say anything at all? The problem is how to break through this so-called *hermeneutic circle*.

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[1] "Der Begriff der Lebenswelt [ist] allem Objektivismus entgegengesetzt. Er ist eine wesenhaft geschichtlichen Begriff, der nicht ein Seinsuniversum, eine 'seiende Welt' meint. Ja, nicht einmal die unendliche Idee einer wahren Welt läßt sich sinnvollerweise aus dem unendlichen Fortgang menschlich-geschichtlicher Welten in der geschichtlichen Erfahrung bilden".

[2] "*Verstehen ist (...) die ursprüngliche Vollzugsform des Daseins*, das In-der-Weltsein. Vor aller Differenzierung des Verstehens in die verschiedenen Richtungen des pragmatischen oder theoretischen Interesses ist Verstehen die Seinsart des Daseins".

[3] "Was lebendig ist, ist in der Tat für das gegenständliche Bewußtsein, die Anstrengung des Verstandes, der in das Gesetz der Erscheinungen einzudringen strebt, niemals wirklich erkennbar".

[4] "Das vollendete Verstehen stellt den Zustand einer neuen geistigen Freiheit dar. Es impliziert die allseitige Möglichkeit des Auslegens, Bezüge-sehens, Folgerungen-ziehens usw.".

The answer is that circularity in interpretation need not be vicious, and, indeed, seldom is. Gadamer argues that it can be an ever-enriching process of relating parts and whole. This process often starts with what he calls *Anstoß* (offence): the experience of strangeness, of incomprehensibility. What seemed familiar shows an unexpected side. This triggers off a question. But a question always is loaded with viewpoints and meaning, with a *Vorgriff der Vollkommenheit* (anticipation of perfection). People often have a good *sense* for posing the right question. Thus, the circle can be broken. An answer to a question may not be immediately adequate, but, when the process has started, a provisional answer leads to a revised question, etc. This process does not end with final definitions. "To define is to distrust, (..) and what definition distrusts is the capacity not only of the reader but of conversation itself. Through definition, a word becomes a term: rigid, predictable, and invulnerable to the twists and turns that a word receives both in dialogue and in the history of the language in general" (Weinsheimer, 1985). Rather, a word acquires meaning through its use, its application.

A second problem could be hermeneutics' *relativism*. If knowledge never is context-free, and interpretation is always context-bound, then, it seems, understanding must always be relative. An interpretation can never claim truth in the way a statement in the objectivistic framework can, because "any attempt to explicate the intention or meaning of an action or utterance requires the assumption of an indefinite number of other beliefs and purposes" (Bohman, 1991). However, this criticism only is adequate if these background assumptions put a *finit* limit on the validity of interpretations. Bohman argues that this need not be so: "Being conditioned by social constraints in no way precludes the possibility of valid knowledge emerging within them, any more than the organic constraints on the human eye's ability to see color implies limits about what we may know about the spectrum, or, similarly, the fact that we see within a horizon limits the knowledge gained by visual perception".

From the viewpoint of objectivism, interpretation also implies *subjectivism*. Subjective knowledge cannot be true knowledge. However, according to Kant (Kant, 1963), subjective conditions for the possibility of experience are *enabling* conditions with regard to objective knowledge of *phenomena*, and limiting conditions only with regard to knowledge of *noumena* or things in themselves. Although Kant was more interested in the noumena than in the phenomena, his argument is also valid for hermeneutics. While the formal conditions for the possibility of knowing make it impossible to know all the determinations of an object, this conditioned character does not imply that what we *do* know cannot have objective status (see Bohman, o.c.). From a God's eyepoint of view, it may be possible to know how things 'really' are, for humans, knowledge is always relative to a human point of view. This subjectivity is an enabling condition for meaningful knowledge. Bias and prejudice only become improper if they are beyond criticism. Far from being subjectivist, solipsist, or skepticist, the thrust of hermeneutic philosophy is to show that more accounts are 'real' and 'true' than is acknowledged by the natural sciences in their objectivist form.

The framework provided by phenomenology and hermeneutics seems suitable to describe and investigate educational phenomena in science education. In the next section, I will evaluate a first attempt to tackle education from this point of view.

3.7 The Working Group Empirical Introduction

Phenomenology is not a new phenomenon in Dutch chemistry education. In searching for a framework that emphasizes understanding, I ran into the work of several Dutch chemistry teachers and educational researchers who eventually gathered under the name of *Werkgroep Empirische Inleiding* (Working Group Empirical Introduction). I will refer to them as the WEI. For some reason, the members of the WEI never elaborated their framework in philosophical terms. I regret this, for it is at the level of philosophy that their approach seems incompatible with the dominant objectivist strand in chemistry teaching. It is clear to me that the philosophical roots of the WEI lie in phenomenology. In this section, I will present the most important ideas of the WEI, after which I try to reconcile their approach with hermeneutics.

Roest: Immediate experience

As early as 1931, the chemistry teacher J.F. Roest expressed his dissatisfaction with the emphasis on transfer of factual knowledge in the secondary school curriculum (Roest, 1931). According to him, development of an understanding of chemical concepts should not take place through statements in a book, which are then illustrated with some facts, but through experience. The role of the teacher is to promote the students' conceptual development but not to drill specific routines. He proposed an inductive-empirical approach in which the contents should be chosen in such a way that students would be guided to understanding, instead of choosing contents for reasons of chemical logic only. In his view, understanding can only be achieved through *immediate experience* of phenomena (Roest, 1968).

De Miranda: Issuing discourse

Roest inspired one of his former pupils, J. de Miranda, to investigate systematically the possibilities for a new approach to chemistry teaching. De Miranda criticized chemistry education for only trying to be accurate with regard to the *results* of chemistry, at the cost of being accurate with regard to the *methods* of chemistry. In his opinion, the teaching of chemistry–the explanations, the demonstrations, the transmission of knowledge in general–showed little resemblance with what chemists really do. He thought it was more important for students to know *how to learn*, that is, understand how to create new chemical knowledge, than just to know the current *facts*.

In 1955, De Miranda (De Miranda, 1955) published a thesis on chemistry education that shows strong influence of the ideas of the Dutch phenomenological psychologist M.J. Langeveld. When dealing with human beings, De Miranda wanted to avoid the positivistic methods of the natural sciences. He therefore distinguished sharply between particular, singular objects, like this book, and universal objects, like books in general. He quotes Langeveld: "The singular object cannot be reached by the sciences, which exclusively deal with universal laws and concepts. The sciences can only deal with collections of objects, with exemplars from classes, with units from collections, which are in principle countable, ponderable, measurable, because they are build up from elements that are identical in nature" (Langeveld, 1950), p. 233, my translation). De Miranda suggests that, to deal with singular objects, we have to employ the methods of the *Geisteswissenschaften*. The potential for understanding the words and actions of our fellow human beings is not grounded in a comprehensive description of humans as mere objects, units of the class of human beings. Our understanding is from inside, because we feel and experience in the same way as our fellow-subjects. The educational situation, then, should not be approached with the methods of the natural sciences, for each educational situation is a singular, not a universal, object, determined by interactions between subjects. According to De Miranda, the objects and phenomena (issues) that are talked about in classroom have the same singular character. This notion was foreshadowed already by Roest (1931, o.c.). Things, which to him were identical, were not always seen that way by students: "A student–working on paper– lets NaCl precipitate. Question: 'Is it insoluble?' He starts thinking and remembers a rule, which says that all chorides are etc. He is told that he undoubtedly knew that salt from the kitchen dissolves very well, and he will feel dumb. However, the mistake is made by the instruction, which has been such that salt from the kitchen and NaCl remained *different things*, notwithstanding the fact that their being identical had been mentioned by the book and by the instruction" (my translation, my italics).

Observations like this inspired De Miranda to reflect systematically on how phenomena exist in educational situations (De Miranda, 1962). The participants–teacher and students–are trying to communicate with each other. They refer to something, for example a piece of burning magnesium which in the objectivist framework must be the same thing, but which nevertheless is experienced in different ways, because everybody sees it in the light of his or her previous experiences. The teacher, for example, interprets the process as a chemist and talks about the chemical reaction in which magnesium oxide is formed. For a student, the product of the process is the blinding flash of light, rather than the unimpressive heap of white ash which remains. Are they talking about the same issue, the reaction of magnesium? De Miranda suggests that problems in learning can arise when the participants in a discourse, who seemingly refer to the same issue, in fact do not have that issue in common. Their way of experiencing and speaking may be so different that they cannot understand each others point of view. In this way, communication and learning can be blocked. When this can be the case even when every participant has *im*mediate experience of the phenomena, it will certainly be so when knowledge of objects is mediated through statements in books.

To help the student learn the objects and phenomena of chemistry, that is, to learn to see from a chemical point of view, the teacher should know the point of view of the student. How does the student experiences the phenomenon, and which meaning have the words the student chooses to describe? Only then will it be possible to guide the student. The teacher should not just try to explain the way chemists interpret the phenomena, in words which are chosen to be correct with respect to current chemistry. De Miranda called this '*zakelijk gesprek*', which I will translate with *issuing discourse*. In an issuing discourse, both teacher and students should try to understand each others understanding, in such a way that a common issue comes into existence. Language plays an important role in such a discourse, since it is in language that experiences are articulated.

H.H. ten Voorde, a student of De Miranda, emphasized the autonomous position of De Miranda's approach with respect to pedagogy and psychology. In his opinion, this teaching is neither the objectivist transmission of content-specific knowledge that characterizes many *chemical* approaches, nor the general cognitive skills development that characterizes many *psychological* approaches; it is the common construction of meaning on themes that are relevant to the group (Ten Voorde, 1977). This is what I would call a *hermeneutic* approach.

Ten Voorde: Levels in argumentation

Ten Voorde developed and applied this approach further, using the theory of *levels in argumentation* as proposed by the mathematician P.M. van Hiele (Van Hiele, 1986). In this theory, learning starts from a perspective in the *life-world* of the student. In this life-world, students already are acquainted with many things and events, but they are not accustomed to question these things from scientific viewpoints. There is water, and there is ice, but why should one wonder if these are the same or not? Students at first simply do not pose such questions. The first obligation for the teacher is therefore to focus students' attention to processes and objects in their life-world from a viewpoint not common to them. If this succeeds, the students are said to be in a *ground-level*. The characteristic feature of this ground-level is that reasoning is still absent. Observations can be made and verbalized, but there is no possibility to argue about statements. One pupil may say that water and ice and steam in fact are the same, another may deny this, but they cannot explain to each other why they think this is so. They lack a common frame of reference. Such a frame of reference can be found when more than one experience is verbalized, and regularities are observed. For example, it may be noticed that when magnesium is brought in contact with steam, a gas evolves. The same gas evolves when magnesium is brought in contact with liquid water. This is an argument that water and steam, from a certain point of view, are the same. When students are able to argue like this, they have reached the *descriptive level*. Argumentation in this level depends on descriptions of experiences. That is, in this kind of issuing discourse the issue, the object of experience, is the similarity in the descriptions. This object does not exist in the ground level, therefore, students who have not yet transcended to the descriptive level are unable to participate in this discourse. They do not understand what is being talked about. Eventually, students may experience a principle that guides these descriptions. Water and steam can be said to be the same not only because they happen to behave the same, but this sameness of behavior can be seen as a necessary consequence of water and steam sharing a fundamental principle: their elementary structure is the same. From this point of view, they *are* the same. In this *theoretical level*, the life-world differences between steam and water have become completely irrelevant.

According to the WEI, it is important that learning takes place along the lines of these levels. It certainly is possible to tell students right away in a process of transfer of information about the categories and theories and models of chemistry, but this will only lead to rote learning. Through drill and practice, students will be able to use the information in a limited set of situations, but they will be unable to transfer this ability to situations that are outside the training situations.

Roest and De Miranda founded the WEI in 1963. Ten Voorde, who participated from the beginning, described the development of thought in this group, their attempts to reform secondary school chemistry teaching, and their framework for studying chemistry education in his 1977 thesis (Ten Voorde, 1977). During the 1960s the WEI developed a new secondary school curriculum along these lines, which was used by a minority of schools in the Netherlands. Ten Voorde describes the classroom research that led to this curriculum and the conceptual developments that proved possible. However, the national policy of unification of curricula and assessment disfavored pluralism, and the WEI lost its position: their curriculum is no longer in use. But their framework for chemistry education–which has proved fruitful in empirical educational research–still is valid.

Implications

In the approach of the WEI, the concepts of immediate experience and issuing discourse play a fundamental role. It is through experience that attention is drawn. It is through discourse that frameworks of reference are developed, to enable understanding of and agreement on observations, experiences and issues. Language plays an important role, since it is in this medium that students express themselves. The switch of level of argumentation can be used as an indicator for learning: if a student does not provide arguments but only delivers statements about her or his experiences, then this is an indication for a ground level; a student who is arguing by referring to other descriptions can be said to have learned, even when the arguments are not immediately correct from the current chemical point of view. However, I found it too intricate to apply this level theory. Understanding is a process that can occur without changes in level, whereas on the other hand descriptions in terms of levels refer to a state a student is in, and not to a process. I choose to focus on the process. Thus, I think that *interpreting issuing discourse is a tool for investigating understanding.*

In the WEI's model of issuing discourse it is not the object itself that comes first. It is the mutual and conscious experience that is the starting point of discourse. Experience has priority. In this respect, the WEI follows the phenomenological tradition: humans do not see or grasp things in themselves, they have experiences which enable them to infer to objects. And it is the context as much as the object itself that is responsible for the characteristics of experience. Learning therefore cannot disregard experience. Students bring their own previous experiences with them, and their way of experiencing the phenomena and explanations that are presented during instruction will have a strictly personal component. As a result, knowledge and understanding will be personal and subjective too. In order to reach *common* understanding, the participants have to explicate their experiences in language. In such a discourse, they may become aware of differences in points of view. Sometimes, these differences cannot be bridged, but in other instances, mutual understanding can occur. This latter process is accompanied by characteristic exclamations as "Now I see what you mean", or, in De Miranda's terms, "Now I understand how you see this issue". This is an experience in itself, an experience of mutual and explicit understanding. The object of experience is no longer a chemical phenomenon; it is the awareness that the object is seen within a certain framework. The things said about the chemical phenomenon now are part of understanding: a meaningful description of one's conscious experiences. *This common understanding as it is explicated in issuing discourse can become the phenomenon for educational research.*

When instruction only provides the chemical phenomena and the correct explanations it does not induce this process of mutual understanding. It is then left to the students themselves to bridge the gap. Moreover, the educational phenomenon of understanding cannot be studied. Thus, a consequence of using this approach is that the educational situations to be studied must allow for issuing discourse.

3.8 Hermeneutics and science

In the previous sections, I have introduced the hermeneutic framework but I have not yet answered the question whether hermeneutics is applicable to *science*. This question can be put differently: is science a form of interpretation? Does the capacity for interpreting and for attaining common understanding belong to the professional qualities of the organic chemist? The recent history of philosophy shows a shift in this direction. Until recently, philosophers defended one out of two positions (Taylor, 1980). On the one hand were those–notably the logical positivists–who wanted to subsume all activities worth being called scientific under the umbrella of the objective method of the natural sciences. On the other hand were those who suggested that the so-called *Geisteswissenschaften* were different. These fields, such as the study of art and history, tried to remain free from the methodological attacks of the natural sciences by appealing to interpretation. It was maintained that works of art and human deeds need interpretation, because they are intentional. In the humanities, one does not only want to know what happened, and how it happened, but also why it happened. Intentions are absent in nature, because intentions require a subject, whereas nature is the objectively given. So, nature is not in need of interpretation. Perhaps the way scientists investigate phenomena can be seen as interpretation, but in that case the humanities consist of a double interpretation. According to Gadamer, history has no 'objects of research' as the natural sciences have: "Ideally, it is possible to characterize the object of the natural sciences as what is known when we will have a completed knowledge of nature. However, it makes no sense to talk about a completed knowledge of history. Therefore it is also not possible to talk in this way about an 'object as such' to focus research on" (Gadamer, 1986), p. 290[1]).

Gadamer has developed his philosophy in this context, to defend truth-claims that are made by the Geisteswissenschaften. His aim was to show that the methods of the natural sciences cannot and should not be applied to art, law, history, or theology; but that these fields have their own access to reality and truth. However, Gadamer holds that *all* understanding is interpretation; hence, the sciences do not have a privileged way of knowing. On the one hand, science depends on the intentions and viewpoints of the scientists, on the other hand, works of art or history contain the same kind of truth as facts of nature, in as far as they show an understanding of the world in which we live. It is interesting to note that Gadamer reverses the attack: not only is it not true that the Geisteswissenschaften are–merely–subjective and personal interpretations, the natural sciences essentially are interpretive too. They have no privileged access to reality, but are as dependent on viewpoints, contextual interpretation and consensus as art and history. This opens the possibility to subsume the natural sciences under hermeneutics.

If science is interpretation, then what counts as a good interpretation depends on the nature of the questions asked. Aristotle, for example, argued that things can be understood in terms of their purpose or function, that is, in terms of *final causes*. To Aristotle, the purpose of a thing *causally* determines the material it is made from. For example, a statue is made of marble because marble is a beautiful and durable material. This is quite a different rendering of causality than is given by modern science (Lindberg, 1992). In the

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[1] "Während der Gegenstand der Naturwissenschaften sich idealiter wohl bestimmen läßt als das, was in der vollendenten Naturerkenntnis erkannt wäre, ist es sinnlos, von einer vollendeten Geschichtserkenntniss zu sprechen, und eben deshalb ist auch die Rede von einem 'Gegenstand an sich' dem diese Forschung gilt, im letzten Sinne nicht einlösbar".

study of history, to give another example, causality is linked to intentions. Something counts as a good explanation if acts can be related to–secret or overt–intentions of the actors.

Aristotle, an excellent observer, did not experiment, because in his philosophy true knowledge (episteme) is knowledge of what is universal and exists *invariably*. Experiments can only distort this natural existence, leading at best to knowledge of things in unnatural situations. This was not the kind of knowledge Aristotle was interested in. Modern science has shifted its interests: it does not just observe nature more accurately, but it makes these observations within a framework of explicit and different conjectures about nature, which are meant to enable the disclosure of regularities as the constant factors in an *ever-changing* reality (Tijmes, 1992). Modern science not only is *description* and *explanation*, but also *prediction* and *control*. The last two aspects influence the point of view from which to describe and explain.

In the opinion of Heidegger, Descartes introduced this framework by reducing things in the world to *res extensa*, the property of occupying space. If all other qualities are but quantitative modifications of this extension, it becomes possible to investigate material things with mathematical rigour (Heidegger, 1986), p. 95). Modern science's preference of this kind of causality is motivated by its will to control and predict. Processes are explained by material causes, because this kind of causality allows for prediction and control in a much more exact way than, say, intentional causality. Through research, new areas are constantly developed to extend such control.

Heidegger argues that to do an experiment means to formulate conditions that enable control of a certain relationship based on preliminary calculations. Knowing-as-research asks the world to account in how far and in which way it can be transformed into objective parameters. Research controls things in the world if it is able to compute its future. In post-Cartesian epistemology, only those things count as 'real'. Science-as-research becomes possible if the reality of things in the world is sought in this facticity (Heidegger, 1963). But the world as a whole escapes science.

If science is seen in this way, then the context of scientific knowledge is determined by those practices that help to predict and control: measuring, reproducing, generalizing, cause-effect explanations, formulating and investigating strict hypotheses. Science can tell us the truth about the causal powers of nature, can be getting it righter and righter about how things work, even if there is not just one right answer to how things are (Dreyfus, 1991). Still, the concepts used in science disclose an irreducibly human point of view. Mary Hesse has argued: "It is impossible in studying theories of evolution, ecology, or genetics, to separate a mode of knowledge relating to technical control from a mode of knowledge relating to the self-understanding of man ... [since] the very categories of these theories, such as functionality, selection, survival, are infected by man's view of himself" (Hesse, 1980). Even organic chemistry textbooks sometimes reveal this 'unnatural' viewpoint: "'Simple' compounds are defined here in an unusual but practical way: a simple molecule is one, that may be obtained by four or less synthetic reactions from inexpensive commercial compounds" (Fuhrop & Penzlin, 1994). This definition shows aspects that can only be understood if science is seen in its context of providing for specific human needs.

If even compounds cannot be defined in terms directly referring to nature, so much less is this possible of the scientific apparatus in use: "Every failure and every disturbance of measurement apparatus leading to useless data can be explained with the same laws of nature, that is, the failure of the equipment does not contradict the laws of nature; it just *fails to meet a human goal.* (...) The objects of physics therefore cannot simply be found in nature; they are constructed in the sense that the technical and conceptual construction of equipment enables the scientist to gain specific scientific experiences" (Janich, 1994)[1].

If science is an enterprise aiming at prediction and control, then it becomes clear that 'understanding' in science *must* be seen from this viewpoint too. Scientists (and students) understand nature scientifically when they are able to pose and answer questions in which the material world shows up as predictable and controllable. The 'basic knowledge' and 'basic skills' a student should master to 'learn to experiment' should thus be related to questions of prediction and control. The descriptions, concepts, laws, etc of science are rather not regarded as *referential*–referring to the world as it really is–but as *instrumental*.

3.9 Hermeneutics and science education

Science education for future scientists is a derivative of science because it has to prepare for science and cannot ignore the frameworks adopted by science itself. The hermeneutic analysis showed that those aspects of reality that emerge in science are determined by descriptions and explanations from the viewpoint of prediction and control. Learning to do science consequently is learning what it is to predict and control. This goal sets science education apart from various other subjects like history and philosophy. Natural science is not interested in explanations in terms of, say, intentions: the natural sciences deal with objects that need not be, indeed should not be, understood as self-interpreting (Rouse, 1991).

Objectivism tries to describe reality 'as it really is'. This suggests that such descriptions are not influenced by the point of view: descriptions are not interpretations. It is consistent with objectivism to base science education on a transfer of correct descriptions and explanations. Books state facts and theories and give definitions using the word 'is'. It is not an issue for objectivism to develop points of view from which to describe and explain. Since objectivism is the dominant philosophy, transfer of information is the dominant educational strategy. In a way, the only difference between teaching and learning is direction. Teaching is presenting the information, learning is absorbing the information.
All educators nevertheless empirically know and accept that transfer of knowledge is not always successful. From the objectivist viewpoint this failure has to be explained. Some of these explanations are related to the learner: lack of motivation, short-term memory overload, inaccessibility of metacognitions, confusion with other concepts, lack of cognitive maturity, lack of previous knowledge, etc. Many attempts have been made to improve science education by taking into account these learner-based variables. In the same spirit, teacher-based variables (teaching styles, teacher cognitions, use of technology)

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[1] My translation of "Jeder Defekt und jede Störung eines Meßgeräts, das damit keine brauchbare Meßdaten liefert, kann im selben Sinne mit 'Naturgesätze erklärt' werden; d.h. die Fehlfunktion eines Meßgeräts steht nicht im Konflikt zu Naturgestetzen, sondern *verfehlt* lediglich *eine menschliche Zwecksetzung.* (...) Die Gegenstände der Physik sind demnach nicht einfach in der Natur vorfindliche, sondern 'konstuierte' in dem Sinne, als es erst die technischen und begrifflichen Konstruktionen von Geräten sind, die dem Naturwissenschaftler erlauben, spezifisch wissenschaftliche Erfahrungen zu gewinnen".

and social variables (group effects, cultural background) have been identified and used to improve the basic process of transfer of knowledge.
For instance, an often-used distinction is between so-called declarative knowledge and procedural knowledge. Declarative knowledge is the content, procedural knowledge (or: skills) deals with how to handle this content and/or how to obtain content. Domain-specific procedural knowledge for example is knowing how to perform a distillation or a titration; general procedural knowledge is on how to obtain data as such or how to solve problems. These skills are additional, that is, you can have declarative knowledge like being able to tell that you can make ethyl acetate from ethanol and acetic acid in the presence of sulfuric acid without having any idea how to perform this synthesis.
According to objectivist teaching, these domains of declarative knowledge and procedural knowledge can be dealt with separately. Problem solving strategies can be taught in a general way and can be applied to all kinds of content. According to hermeneutics, this is not possible. In the first place, the term 'declarative knowledge' has no proper meaning apart from the procedures necessary to construct that knowledge. To understand a proposition one also must have an understanding of the context from which the proposition derives its meaning. This implies having enough experience with a certain context to be able to interpret and apply. If you do not know how to react ethanol and acetic acid to make ethyl acetate, than you do not understand what 'to react' means in this context, which implies that you do not understand the proposition. Procedural knowledge is not optional; it is necessary.

This also implies that general procedural skills in isolation from a context do not mean much (Lijnse, 1994). A student who can solve problems in a few areas of chemistry can be called a good problem solver, but this does not necessarily mean that she or he will have competence in yet another area. If understanding is contextual, it will be difficult to transfer competence in one context to another context. This hampers the possibility to speak in general terms about students' competence, notwithstanding Corey's statement I quoted in section 2.4.2, where he advocated that students should apply "general problem-solving techniques". For example, a student may acquire considerable competence in acid-base chemistry, being able to apply her or his understanding fruitfully in making buffers and determining concentrations. Such competence could then be described in terms of general problem-solving skills. However, this competence does not transfer to another area of chemistry, in which the same student may be virtually helpless, notwithstanding a proven ability for these higher order skills. Terms describing knowledge, competence, skills and understanding can only be used fruitfully in relation with a specific context. Hence my preference to designate learning with the term *contextual development*.

Information can be 'known' without experience in the relevant context. "(...) discourse which is communicated can be understood to a considerable extent, even if the hearer does not bring himself into such a kind of Being towards what the discourse is about as to have a primordial understanding of it. We do not so much understand the entities which are talked about; we already are listening only to what is said-in-the-talk as such" (Heidegger, 1962), p. 212[1]). Heidegger has called this phenomenon 'idle talk': "Idle talk is the

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[1] " (...) kann die mitgeteilte Rede weitgehend verstanden werden, ohne daß sich der Hörende in ein ursprünglich verstehendes Sein zum Worüber der Rede bringt. Man versteht nicht so sehr das beredete Seiende, sondern man hört schon nur auf das Geredete als solches" (Heidegger, 1986), p. 168.

possibility of understanding everything without previously making the thing one's own" (p. 213)[1]. This is meant in a technical sense rather than contemptuously. It is not in itself wrong only to be able to reproduce what is written in textbooks, for example, it enables people to enjoy the scientific pages in the newspaper. It gives people a sense of scientific literacy, which is necessary to appreciate the culture we live in more fully. But if this phenomenon signifies something positive, it is in the area of 'knowing *about* science'. This is not per se a sufficient preliminary for *doing* science.

A different attitude towards this is displayed by Martin Eger, one of the very few educational scientists relating hermeneutics to science education. He differentiates between what he calls the Book of Nature and the Book of Science (Eger, 1993). The Book of Nature is written in a specific way, in the form of the results of research. You can only understand this book if you understand something of the scientific enterprise. Eger therefore suggests that students face a double interpretive task: in order to be able to interpret and understand the Book of Nature the way scientists do, they need to be able to interpret and understand the Book of Science: "The idea that true interpretation inheres only in the composing of the book of science, not in its reading, derives from the common belief that although raw data does need interpreting, by the time the results reach the textbook all interpretation must surely be over. (...) The line between receptive and creative interpretation–between *finding* the meaning and *constructing* the meaning–cannot always be drawn". Although I agree with this, his analysis of hermeneutics as an approach to science education seems to ignore the influence of the context on meaning. He rejects the possibility of direct transfer, and emphasizes the fact that students have to interpret, but they still have to interpret propositions, and not experiences. I prefer to emphasize the differences between learning about science and learning to do science. I doubt whether learning the book of science (learning about science) is sufficient to understand the book of nature in the sense that participating in scientific research becomes possible. Interpreting the book of science may be the right thing to do if learning *about* science is the goal. However, students of chemistry should be able to *do* science.

According to my view on science education, transfer of information can *not* be the basic process. Understanding is central. The paragon for science education is scientific research itself, in which scientists, ask questions, interpret their experiences, come to an understanding, apply it, and finally explicate this understanding in the form of knowledge. Science education necessary takes place in a context, since understanding is not intrinsic to words and propositions. Language gives meaning to experiences with things and events in a specific context; this meaning consequently depends upon the experiences. To understand, it is necessary to adopt a point of view within the context. It is not sufficient that a teacher tells a student from what point of view certain propositions have been constructed. Transfer of viewpoint is not possible. Language and discourse consequently have a different and more important role to play than in objectivist-style transfer of knowledge. In objectivism, words simply *have* meaning because they refer to things in the world. In hermeneutics, words have to *acquire* meaning through interpretation and discourse, which happens in language.

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[1] "Das Gerede ist die Möglichkeit, alles zu verstehen ohne vorgängige Zueignung der Sache" (o.c., p. 169).

Of course, science education cannot be identical with scientific research, if only because it would take a lifetime to construct insights that are currently considered to be basic to science. There is no time to repeat history. There is no point in following all the detours and blind alleys. Moreover, the goal of science education is not to give opportunity for a fresh start. Students are supposed to catch up with *current* interpretations, perhaps not in an uncritical manner, but they should not invent a different science. It follows that I have to find a middle road between re-enacting science and transfer of results.

Transfer of *knowledge* is incompatible with a strict hermeneutic interpretation of knowledge and understanding. But it seems to me that it is possible to give transfer of *information* a proper place when certain conditions have been met. When learners already are acquainted with the context of the additional information, transfer can be successful. Scientific conferences often succeed in transferring information because the participants of such meetings share the same understanding drawn from research experience within a shared domain. They also usually share a commitment to the same points of view and they have an interest in the same questions.

Information transfer can be successful in education, too, if the basic concepts needed to interpret the information are already understood by the learners, and if the new information to be transferred does not change the meaning of these concepts too much. However, understanding cannot be transferred. It may take several years to see certain phenomena with the eyes of a scientist, but then it is no longer possible to see it from a layman point of view, or from the point of view of a student. It is the universal experience of the expert that he or she cannot understand why others do not see what is so obvious. *This implies that a reconstruction of expert knowledge is not the way to structure teaching when understanding should take place.*

It remains a question which experiences, discussions, interpretations etc. are necessary for understanding to occur. If this would be known, it can be deduced when transfer of information becomes appropriate. Once more, experts' reconstructions are of little help, since they already presume understanding. A reflecting expert may remember several instances that were revealing to him or her, but such an introspection is not systematic. Since there is no theory whatsoever available to predict what is necessary for understanding, the question still is an *empirical* one.

4 Methodology

4.1 Hermeneutics and research in science education

Doing *research* in the field of science education, and answering the empirical question indicated in the previous chapter, implies a methodology. When the object of my research is the *historic* phenomenon of understanding, it follows that a methodology has to be adopted that does not try to make understanding into an scientific object for prediction and control. Does that imply that hermeneutic methodology can only yield impressionistic case studies without any further relevance or claims to truth?
I do not think that is the case. The fact that all understanding is historic does not lead to the conclusion that all educational situations in which understanding occurs are unique in the sense that nothing of a more general nature can be said about them. Uniqueness is not the issue. Each sugar crystal is unique too, still, many true things can be said about sugar crystals in general. Likewise, many true things can be said about educational situations in general. However, "Interpretation of historic objects goes back to primary entities that are not data of experiments and measurements, but units of meaning" (Gadamer, 1986), p. 71[1]). Historic concepts–including those that interpret how students understand–are meant to give *meaning* to specific events, not to *measure* these events. Educational events–and understanding is such an event–can be understood using context-specific concepts. The theory of levels of Van Hiele/Ten Voorde can be seen in this light. There is no specific hermeneutic reason to analyze discourse in terms of the presence of generalized descriptions or causal theories; its usefulness lies in the fact that such descriptions and explanations constitute science by providing the means for prediction and control. If students start describing events and experiences in a generalizing way, this can be taken as a sign of scientific understanding. That is, the students start to construct objects and concepts which are meaningful in a context of prediction and control. The transfer to the objectivist framework is made when the word 'meaningful' is replaced by the word 'correct'. 'Correct' is related to the results of understanding, which are objectified and lifted out of the context. Understanding is never 'correct' in this sense, although in moments of understanding a person can have a strong feeling of being right.

Understanding is disclosed in application, hence, in what someone does or says. If (speech) acts are fruitful and sensible in the specific context, they can be taken as a sign of understanding. A teacher can base his or her activities on the development of students' understanding. The educational researcher should try to explicate both the students' and the teacher's understanding in words. This may be taken as an objectification, introducing the possibility to set up categorization schemes for scoring understanding. However, this would overlook the fact that such a categorizing itself is also a moment of understanding, taking place in history. It is possible to talk sensibly about understanding in terms of chemical educational concepts, but these concepts are historic, and not objective. That is, they can only be applied in a historic context: to interpret a concrete educational situation. What 'understanding chemical equilibrium' means cannot be separated from how the

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[1] "Die primären Gegebenheiten, auf die die Deutung der geschichtlichen Gegenstände zurückgeht, sind nicht Daten des Experiments und der Messung, sondern Bedeutungseinheiten".

student acts (in words and deeds) in the context in which chemical equilibrium is presented to her or him as a phenomenon. In a calculation question ('calculate the equilibrium constant of ...'), chemical equilibrium is presented in a different context than in the aspirin synthesis. Consequently, understanding equilibrium in the first context is not the same as in the second context. Categorizing understanding across contexts or even without taking contexts into account thus is meaningless.

Whereas the student can turn his or her understanding into chemical objectifications, the educational researcher cannot do this. "Certainly it is possible to derive general rules of experience from historic experience, but their methodological value is not the same as that of a law that would apply to all occurring cases without ambiguity. Rather, rules of experience demand having had experience in practice; they essentially are what they are only in such practice" (o.c., p. 246[1]). Consequently, tools for interpretation are not suited to objectification. They do not measure objectively, like a thermometer, which measures temperature without understanding or knowledge of the context. Someone has to take the decision that it is appropriate to measure temperature in that context. Such a judgment relies on understanding.

Interpretation thus can follow rules, but these rules cannot have the exact character of prediction and control as scientific rules have. Gadamer compares hermeneutic rules with *phronèsis*. Phronèsis is the kind of knowledge linked to practical decisions. It is the form of reasoning which mediates between general rules and what to do in particular situations. The term belongs to the philosophy of Aristotle, who used it to denote *practical wisdom*. "It deals with that which is variable and about which there can be differing opinions. It is the type of reasoning in which there is a mediation between general principles and a concrete particular situation that requires choice and decision. (...) Such choosing is a rational activity, although the reasons to which we appeal do not necessarily dictate a univocal choice" (Bernstein, 1983), p. 54). Understanding is knowing how and when to apply certain rules and maxims. These judgments themselves are not based on rules or algorithms, but they are learned through experience and practice. It is only through application that becomes clear what rules mean. Both students of chemistry and educational researchers have to learn this. Students of chemistry have to learn how to apply chemical rules, laws, theories and data to specific situations. That is, they should learn to interpret. Learning to do research is learning to discover, understand and apply the concepts that govern organic synthesis.

Learning to do (this kind of) educational research is developing appropriate interpretations, that is, to see an educational context from a viewpoint from which the acts and words of the students appear to be meaningful. *The educational researcher is in a hermeneutic situation analogous to the student's situation*, who is in a chemical context and tries to make sense of chemical experiences. Both try to understand. The students tries to understand chemistry, the researcher tries to understand the process of teaching and learning chemistry. Both can check the validity of their understanding only on their applications. The difference is that the students' understanding can be made explicit in the interpretations of the researcher, whereas the researcher cannot explicate his or her own understanding. That would take a viewpoint outside oneself. The understanding of the

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[1] "Gewiß kann man aus geschichtliche Erfahrung allgemeine Erfahrungsregeln ableiten, aber deren methodischen Wert ist nich der einen Gesetzerkenntnis, unter der sich alle vorkommende Fälle eindeutig subsumieren ließen. Erfahrungsregeln verlangen vielmehr einen selbst erfahrenen Gebrauch und sind im Grunde nur in solchem Gebrauch, was sie sind".

teacher is relevant, too: when the teacher understands how students learn chemistry, this learning process can be facilitated.

Having said this, I could continue with directly turning these reflections into specific methods and techniques, and start empirical research. However, many attempts have already been made to study science education. It would be foolish to ignore these approaches. In chapter 2, I describe several attempts to deal with the cookbook problem from a content-specific but objectivist (chemical) point of view. In the next sections, I analyze a few prominent general process skills (psychological) approaches to research in science education. In section 4.7 I will return to the hermeneutic approach again.

4.2 Constructivism

Nowadays, *constructivism* seems to be the dominant paradigm in research in science education (Bodner, 1986; Duit, 1990; Von Glasersfeld, 1989). Current theories on conceptual change and concept mapping very often refer to constructivism as the underlying philosophy. According to constructivism, knowledge (or understanding) has to be *mentally* constructed by the learner. One of the reasons for constructivism to denounce the naive transmission of information model is because this too much resembles the crude stimulus-response ideas of behaviorism (Jonassen, 1991). The proposition is the stimulus, and students' reproductions on achievement tests are the response. Knowledge is not simply the response to an instructional stimulus; the learner has to process the information internally to turn it into knowledge. "One could be a full realist about the external world and even an epistemic optimist about the possibility of knowledge, yet, in the next breath, claim that it is pointless just to shovel extant knowledge into a child's brain because such 'force feeding' *won't* result in that knowledge being internalised and becoming part of that child's interpretive framework" (Matthews & Davson-Galle, 1992). Superficially, constructivism has many things in common with hermeneutics, but there are some differences. Constructivism is not so much a philosophical as well as a *psychological* theory. It focuses on cognitive processes–on how the students think–and tries to detect categories with which to describe this thinking. This tends to deflect attention from *what* is taught and *how* it is taught. Many constructivists do not seem to reject an objectivist framework. Consequently, they suppose that the format in which content is presented to students matters only in as far as it helps or hinders the mental processes of the students. Constructivists think that transfer of knowledge often does not *work*, but not that such transfer also implies that different meanings come into being.

According to hermeneutics, meaning is not something inherent to knowledge. It is the context that determines the meaning. Objects, processes and concepts do not exist prior to experience, interpretation, and verbalization in language. Thus, the educational context deserves as much attention as individual students' mental processes. Teachers and curriculum developers also need to be constructivists: they have to acknowledge that 'force feeding' the chemical content into a curriculum won't result in a curriculum that makes sense.

Moreover, the medium of understanding is language. The way students understand is disclosed by their acts and words. To the study of understanding, it is not necessary to make mental processes an issue. Instead of focusing on short term memory or left and right brain hemispheres it is far more important to analyze science and scientific practices to find out how meaning is constructed there. This also implies less emphasis on individuals and more on group processes, since meaning belongs to the group of users of a specific language. In summary, constructivism often is constructivist only with regard to the learner, not with regard to scientific knowledge itself, nor with regard to the educational context.

Thus, the hermeneutic framework points in a different direction than the constructivist framework. It focuses on *group processes* instead of on individual learning, on *discourse* instead of on thinking, on *contextual development* rather than on presenting information.

4.3 The cognitive approach to laboratory education

In chapter 2, I described several attempts of chemistry instructors to solve or circumvent the cookbook problem. Not only chemistry instructors have paid attention to this problem, educational researchers with a background in social sciences have done the same. There are some noticeable differences.

Scientists in general teach as they have been taught and as they think they have learned (Trumbull & Kerr, 1993). The Utrecht Curriculum provides an example. First, chemistry is divided according to classic fields: organic chemistry, inorganic chemistry, physical chemistry, biochemistry, etc. Each has its own professors, which determine the contents of the courses. Second, a division is made into what is called theory (the lecture courses) and practice (the lab courses). Chemistry instructors organize their teaching on the basis of their chemical knowledge. They seldom make use of educational theory. Nevertheless, some echoes of the results of educational research have permeated into the chemistry curriculum. Chemists have learned to distinguish between knowledge and skills, and to talk about objectives not only in chemical terms, such as 'students should learn nucleophilic substitution', but also in a generalized, non-content specific way. The Utrecht curriculum, for instance, mentions that students should learn "to observe properly in self-conducted experiments".

Bodner writes about science instructors: "David Ausubel proposed a rule that can be summarized as follows: The best way to organize information after it is understood is not always the best way to organize it so that it will be understood in the first place. The organization of our courses seems logical to us, because we understand the material. But that doesn't mean our courses are organized in the optimum psychological order for someone encountering the material for the first time" (Ausubel, 1963; Bodner, 1992). Ausubel's dictum indicates that an approach that is discipline centred does not provide criteria for the construction of a program; instead, we must search for a psychological order.

This line of research that searches for a 'psychological' order and focuses especially on such general skills as 'observing' is called the *cognitive* approach. Its basic supposition is that general procedural skills correctly comprise what scientists do and what students have to learn and are more useful than the content-specific way experts describe their field. "Most cognitive psychologists assume that all resources for solving problems are located in the reasoner's head. This individual has available specific declarative knowledge and a range of procedural skills that aid in the solution of a problem. (...) A range of procedural skills are thought to be domain independent" (Roth, 1994). Another important supposition is that any context consists of building blocks that can be isolated and transferred without changing their meaning significantly: “Transfer happens when a new context or purpose shares elements with an old learning context or purpose” (Butterfield & Nelson, 1989).

Educational researchers seldom pay attention to higher science education. This is somewhat strange, since if it is true that learning chemistry shares many elements with, say, learning to compute, one would expect an application of these findings. In a recent study, Kirschner investigated practical science instruction using the cognitive paradigms (Kirschner, 1991). I think it is worthwhile to follow his line of thought for a while. Kirschner also criticizes the traditional laboratory courses, but he draws very different conclusions. He writes: “... many leading educators and scientists [have] the assumption that scientific knowledge can best be learned through experiences which are equivalent to or based on the procedures of science. This led to a commitment of educators to extensive laboratory work and the use of discovery and enquiry methods of learning. The basic error here is in assuming that the pedagogic content of the learning experience is identical to the methods and processes of the discipline being studied” (o.c., p. 34). According to Kirschner, the stress should be on the *syntactical structure* of science: “those thinking and reasoning skills used by academics within the different disciplines of the Natural Science” (p.34). These skills should be taught before a student can engage in science itself. Citing Hurd (Hurd, 1969), Kirschner rejects structuring science education according to the rationale of the scientist. “According to this rationale, the teaching of science should reflect the nature of science as it is known to scientists and should embody the specific characteristics of the discipline it represents. Disciplines have a conceptual structure identifying the knowledge of which they are composed as well as particular modes of enquiry, that is ways of gathering information and processing it into data. The methods are disciplined with ‘ground rules’ governing the processes. The rationale of the scientist holds that a science course should be a mirror image of a scientific discipline, with regard to both its conceptual structure and its patterns of enquiry” (p. 34).

Kirschner apparently rejects traditional lab courses because they are modelled after science. He proposes to teach how to discover first, and he seems to believe that transfer is possible from general problem solving skills to doing research. As a proponent of distance learning, he advocates curricula that teach how to do research without actually engaging students in the laboratory. He argues that this must be possible, since ‘practicals’ that teach through film, audio, (interactive) video, and computer simulations can teach students these general and specific skills just as well.

Kirschner rejects the structuring of science education after science because the student is not a scientist: “If students are ever to discover scientifically, then they must first learn both the content as well as how to discover!” (p. 36). He therefore needs to characterize this syntactical structure of science in generic how-to-discover-like terms and objectives. He found out that he needed to develop these categories himself, since science educators apparently travel on another wavelength: “Attempts to organize the objectives are hindered because the stated objectives are either so detailed that they can only be of use in specific laboratories in specific disciplines or are so general that they include almost anything one can think of, for instance imparting information, training basic processes and building up adequate motivation. More than 100 different specific objectives for science practical work were catalogued and subsequently divided into six, student-centred general objectives”. These objectives are reproduced in Table 4.1.

In Kirschner's opinion, "one should start by formulating general instructional objectives. These objectives are consequently redefined in more specific, behavioral objectives" (p. 28). He lists 64 specific objectives. Examples are 'to understand the purpose of an experiment', 'to collect experimental data', and 'to assess relevance of experimental data with regard to a hypotheses'.

Table 4.1 *General objectives of practicals in higher science education*

A	To solve problems (including the formulation of hypotheses).
B	To use knowledge and skills in unfamiliar situations.
C	To design (simple) experiments to test hypotheses.
D	To use laboratory skills in performing (simple) experiments.
E	To interpret experimental data.
F	To clearly describe the experiment.

Kirschner shows that laboratory instructors agree with this way of describing, redefining and subdividing their lab courses; at least, they validated his lists of objectives by answering questionnaires, in which the instructors could indicate which objectives were present in their courses, and how they would rank them. Nobody seemed to object that this is the suitable framework to describe the things taught and learned in lab courses.
In the same spirit, others have developed tests and programs to test scientific thinking, problem solving, conceptual thinking, and so forth. When such tests are applied to evaluate laboratory instructions, they often reveal that students who have received laboratory training do not perform significantly better. In this respect, the very limited study of Yager is always cited (Yager, Engen, & Snider, 1969). These outcomes sometimes are used as an argument against laboratory teaching.

I agree that it is possible to criticize current science teaching. However, I do not accept the analyses and solutions of the cognitive approach. In chapter 3 I argued that it is not possible to isolate skills from their context, teach them in another context, and end up with students knowing how to use these skills in the original context. There is ample evidence that knowledge is contextual. "Because all processes are theory-impregnated, and are inextricably linked with other processes, it is not possible to engage in theory-free investigations or to develop skills of observation, data collection, classification, inference, and so on, in isolation. Since one's capacity to use the processes of science effectively is dependent on one's theoretical understanding, it follows that teaching for process skill development is inseparable from teaching for concept development" (Hodson, 1992a).
The meaning of both facts and procedures depends on the context and cannot be isolated without changing their meaning. Roth argues: "Recent ethnographic studies in scientific laboratories revealed an image of scientists that has little to do with the rational reasoner who applies a set of special science process and problem-solving skills. Rather, this area of research has shown that the reasoning of scientists is characterized by its local nature, depending on the research context and on the concrete research situation (Knorr-Cetina, 1981; Latour & Woolgar, 1986). (...) The myth of the scientific rationality and problem solving is established when the scientists strip the contextual factors and report their new constructions as if they were the product of unaltered intentions" (Roth, 1994). It is legitimate that cognitivists pursue their own research program and search for the communal in various activities; however, scientific knowledge depends too much on

domain specific factors. Without situated experience, 'basic' or 'declarative' knowledge remains inert, and 'basic' skills, 'procedural', or 'syntactical' knowledge are vacuous. Accordingly, "teaching methodology must vary with the content and context of theory" (Duschl, Hamilton, & Grandy, 1990).

It is true that chemists have problems constructing a curriculum on the basis of their own conceptual logic. But does the cognitive approach present an alternative? I do not think it is possible to use a list of objectives phrased in general, non-specific terms to construct educational material in any specific sense. Although it is possible to generalize existing situations, the reverse is not possible: there is no route from the general to the specific when one does not know the specific. In the general sense, the objective 'learning to experiment' is present when one-year old children are playing with blocks and when Nobel prize winners are developing new theories. So, to flesh out any curriculum, the cognitivists have to turn to the experts again.

It seems to me that the current problem with lab courses is not that they are modelled after science, rather, it is the opposite. What is called 'experimenting' is in fact skills training, reproducing and ad hoc illustrating. Kirschner seems to believe that cookbook lab courses 'follow the procedures of science'. His rationalized alternative to the lab thus remains based on the same cookbook-like activities. This approach leads to a list of objectives that, although validated by instructors, is not based on accurate observations of the educational processes themselves, nor on an analysis of the professional situation. An instructor might agree in an interview or questionnaire that objectives like 'learning to experiment' are present in the lab course, but a critical observer of the lab course might disagree. Kirschner showed that, when asked about the general objectives of their lab course, instructors agree with the 'learning research skills' kind of objectives. Sometimes, the official curriculum documents, like those at Utrecht University, are embellished with such objectives, showing that chemistry teachers have become aware of these ideas. Nevertheless, as my observations show, the actual educational situation can be completely different. Although some chemists have learned to use the cognitivist language, this is not a way of speaking that is natural to them. When the questions are not phrased in terms of cognitive categories, chemistry instructors, it is my experience, rather refer to situated objectives, like: "This experiment illustrates the electrophilic nitration of aromatic compounds. Students learn how to conduct such a reaction, how to control the temperature, and how to perform a vacuum distillation".

Cognitivists, from Ausubel to Kirschner, are right in claiming that experts should not impose their own logic on the structure of the curriculum. A list of chemical topics does not suffice to structure learning. However, they have too little to offer themselves. The important question in chemistry education is not whether objectives like 'learning research skills' should be present: they should. The question is: which *chemical* content and structure help to achieve this goal. *While it may be possible to teach the various cognitive skills required for doing research without really engaging in science, it is unlikely to be successful.* The students will become expert problem solvers in the domain of the training situation only. They will not acquire the understanding that is necessary for doing chemical research.

4.4 Misconceptions and conceptual change

The cookbook problem is not the only problem in science education. A considerable amount of research attention goes to so-called *misconceptions*. Students often use scientific terms in a different sense than the scientifically accepted one. Therefore, *conceptual change* is needed to change these misconceptions (Dreyfus, Jungwirth, & Eliovitch, 1990; Driver, 1988; Fensham, 1984; Fensham, 1992; Gil-Perez & Carrascosa, 1990; Hashweh, 1986; Hewson, 1981; Novak, 1993; Posner, Strike, Hewson, & Gertzog, 1982; West & Pines, 1985; Zoller, 1990). Since this latter term has a negative ringing, some researchers prefer different terms, such as alternative conceptions, alternative frameworks, or preconceptions.

Problems occur especially when scientific terms also occur in daily life. Students, for example, say that a force must be applied to maintain a constant velocity; that energy is something that can wear down; that heat and cold can flow in and out; that something is in equilibrium when nothing happens; that milk is a pure substance; that electric current is used up in a light bulb; that the earth is flat; and that heat comes from moving molecules but that the molecules themselves are cold inside. Such ideas, it is thought, should change because they are wrong. The problem is that science teaching is remarkably unsuccessful in achieving this.

It is felt as a disappointment and as a failure that pupils and students keep believing in a flat earth, in Aristotelian concepts of force, in molecules as tiny pieces of matter, etc., instead of bringing their life-world knowledge in tune with 'how things really are'. According to objectivism, there can be only one 'true' concept of force, of substance, of energy. This problem became more urgent when science teaching began to relate science with society. It was felt that science should not just be taught as an abstract, axiomatic subject without links to normal life. Instead, science teaching should include scientific explanations of daily-life phenomena. However, this connection is often made from an objectivist point of view, which presupposes that everything in life-world contexts can be described, explained, predicted and controlled with the same fundamental entities and principles as are in use in science. From a hermeneutic point of view, this makes no sense. Science is but one context in many. Its descriptions are only meaningful in relation to the prediction-and-control point of view. This is not the point of view from which people normally experience their life-world. "The subdivision of words and issues, which any language conducts in its own way, constitutes everywhere a first conceptualization that is far removed from the system of scientific conceptualization" (Gadamer, 1986), p. 439[1]).

It seems to me that the misconceptions-research usually addresses the problem from an objectivist point of view. It takes a reductionist point of view in thinking that scientific concepts and theories underlie all processes in the world, in the laboratory as well as in any life-world situation. And it may even believe that understanding can occur through transfer of knowledge. However, students cannot *develop* a concept when it is already *presented* to them.

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[1] "Die Aufgliederung der Wörter und Sachen, die eine jede Sprache auf ihre eigene Weise vornimmt, stellt überall eine erste Begriffsbildung dar, die sehr weit von dem System der wissenschaftlichen Begriffsbildung entfernt ist".

From the hermeneutic point of view it is understandable that many life-world concepts are not changed by science teaching. There is no continuum between the life-world context and the contexts of science. In the life-world, other needs and desires prevail, shedding different light on things and events. The point of view is different. Explanation in daily life is not constrained to physical causality. The specific causal viewpoint of science cannot be made understood through transfer. "Natural sciences break with ordinary knowledge by organizing experience under categories that go beyond or are not available to sense perception. (...) In the learning of the natural sciences the problem or question (if there is any) is not the start of the activity of knowing. The 'Have you wondered?' that opens the chapters of some science textbooks is just a rhetorical question to introduce a series of facts and explanations about which the students and the teacher have never wondered and most probably are not going to. Not only the question is rhetorical but the answer is known and is to be found in the textbook, in the teacher's mind or in the library (Bettencourt, 1992)." It seems to me that, to deal with life-world issues, a different kind of chemistry is needed, which does not necessarily starts with scientific concepts like elements and molecules.

If one believes in science as objectively describing reality, then everyday language must be seen as a source of misconceptions, instead of as a way of revealing and expressing truths of a different character. Words like force, energy, and substance *can* have different and incompatible meanings in different contexts. Even in science the meaning of terms can be different in different contexts. For example, the concept of equilibrium in thermodynamics means that the system has maximum entropy compared with all bordering states. In biochemistry, equilibrium means that a system is in a steady state, where influx and outflux cancel each other's effects. Needless to say that the word 'system' also has a different meaning.

The goal of science education should not be to show that life-world meanings ultimately can be reduced to scientific meanings, nor to declare that certain meanings are mistaken. I do not want to follow the misconceptions research when it tries to identify areas and concepts in which unscientific meanings occur, in order to change them. The interesting thing about misconceptions research is that it is content-specific instead of generic. But it is not *context*-specific. Contexts are necessary to give meaning to content. *It seems to me that learning science is 'contextual development' instead of 'conceptual change'.* A hermeneutic approach would allow students to decide upon meaning and changes of meaning themselves.

4.5 Concept Mapping

Many achievement tests in science education tend to focus on propositional knowledge and straightforward calculations, which allow for rote learning. In the long run, this is unsatisfactory, both to the student, who may receive good marks but has no idea what it is all about, and to the teacher, whose insight into students' understanding is obscured. Following Ausubel's distinction between rote learning and meaningful learning, Novak developed a technique called *concept mapping* (Novak, 1991; Novak, 1988; Novak, 1990). The procedure consists of an analysis of a certain context, for example chemical equilibrium, and pinpointing the basic concepts, such as reversibility, Le Chatelier's principle, equilibrium constant. This can be done by a (chemical) expert, if necessary. The students receives a list of these terms or an envelope containing cards with the names of the concepts, and then have to make a 'map' in which they link concepts using meaningful labels. A label is a sentence explaining how the terms are linked. This map can be made at various moments during instruction, and with various purposes: for the teacher, to get information on students' conceptions; for the student, to be a tool to structure the educational material.

I do not think that this approach can suit my needs, though. What bothers me is the problem of selecting the concepts, and the question of what these concepts mean. It is not at all a straightforward task to find and select the concepts that characterize a certain context. There will be many differences between various experts in the way they would draw a concept map of their field, both in the concepts used, in the labels employed to characterize the relations between concepts, and in the meaning of the terms themselves. The idea that an area can be covered by a given set of terms reveals a dominant influence of objectivist philosophy. This way of concept mapping has to be accompanied by a transfer-of-knowledge type of instruction, since this is the only way in which terms can acquire fixed meanings to students. Terms as such have no intrinsic meaning. Moreover, the meaning of concepts depends very much on practical situations, whereas concept mapping is restricted to propositions.

Quite often, the selected concepts do not come straight from somebody's understanding of a given field, but are chosen from a textbook dealing with the field. This is second-hand experience and second-hand meaning, at best enabling students to learn the way textbooks deal with propositions. That can be a good preparation for an achievement test, though.

When students are unacquainted with the context, they cannot select concepts themselves, so they have to rely on a textbook or on an expert's choice. If they have some experience within the field, they can have their own pick, which seems to me to be more in line with a hermeneutic approach. Although that will make their concept maps more revealing, some advantages of concept mapping are lost. One of the reasons to work with a standardized set of terms is to make concept maps comparable, given the presupposition that terms have an intrinsic meaning. If this is given up, *individual concept maps are incomparable because they are different in meaning and point of view*. As a source for educational research they can still be useful, but they have to be interpreted one by one. Since concept maps reflect the teaching and learning process only very indirectly, it is questionable whether such an instrument is efficient. It does not show how and why students came to the interpretation they present in their concept map. A concept map can be a product of teaching and learning, it can be a valuable tool for students to structure their knowledge and understanding, but it reveals little of the educational process in which understanding arose.

4.6 Quantitative or interpretive research

In hermeneutics, interpretation is important to understanding. Does this automatically imply that an interpretive methodology should be used, as opposed to a quantitative methodology? I see no reason to reject a quantitative approach out of hand. In the words of Silverman, "There are no principled grounds to be either qualitative or quantitative. It all depends upon what you are trying to do" (Silverman, 1993). What I am trying to do is to study understanding as it occurs in relation with teaching and learning organic synthesis. Is it possible to quantify this?

"The purpose of quantitative research in science education is to design and complete systematic, unbiased investigations of the relationship between some intellectual, psychosocial, or instructional variable (independent variables) and science proficiency (dependent variables)" (Nurrenbern & Robinson, 1994). Thus, when the relevant independent variables are known and controlled, students' proficiency in science can be predicted. Reversibly, an established measure of science proficiency can be used as a starting point to detect the variables that explain this proficiency. It seems that quantitative research is consistent with the dominant point of view in natural science: prediction and control.

In education, an element of prediction and control clearly exists. Students are supposed to learn chemistry through curricula. If these are adequate, they predict that after some time students will have acquired specific knowledge and capacities. The results are controlled and monitored by tests and teachers. From this point of view, education therefore can be investigated reasonably well using objectivist methods, aiming at optimizing and rationalizing the process. Arguably, this is the dominant trend in research in science education (Shulman, 1986). Within this paradigm, interpretive research is often regarded as a *preliminary* stage, meant to discover relevant variables and categories which then can be quantified objectively.

In order to quantify and to derive valid conclusions, both the independent and the dependent variables need to be determined unambiguously. The variable 'science proficiency' therefore has to be defined with some rigour. Often, scores on standardized achievement tests are used. The same holds for the independent variables. In order to predict and control, the human participants have to be treated as examples of a population. This inevitably reduces them from self-interpreting and intentional actors to objects whose behavior is seen to be causally determined by or at least significantly correlated to the variables. Quantitative methodology is only able to use unambiguous concepts: in order to count, the entity to be counted is not allowed to change meaning. So, a student is a student, an answer is correct or wrong, etc. A statement like 'Seventy percent of the students used the concept of chemical equilibrium correctly' refers to a group-characteristic; it does not disclose much about individual students' understanding.

Since students are not at all identical, sophisticated statistical sampling and correlating techniques have been developed to circumvent this problem and derive conclusions that can be generalized. Here, social science differs significantly from natural science. In science, reduction to sameness of molecules, reactions, etc. is achieved by definition. That is, entities are transformed to a-historic objects. Consequently, experiments in science are seldom repeated. Spreads and uncertainties are caused by insufficient precision within the measurement techniques themselves, not by, say, different interpretations of the molecules on how to react to the probe. In social science, the spread is induced by the 'objects' themselves. Statistical techniques thus serve a different purpose in both areas.

Much research attention is paid to the 'independent variable'. Some measure of science proficiency is correlated to various parameters thought to influence the outcome. Examples of independent variables are gender, teaching style, students' cognitive ability, new teaching material. Some of these parameters, such as gender and age, appear to be unambiguous by themselves; others, such as intelligence, problem solving capacity, attitude towards science, and cognitive level, are themselves social and cultural constructs that need theoretical justification. "Instruments used to measure various intellectual characteristics, such as formal reasoning capability, working memory, spatial ability, and disembedding ability, have been tested and accepted as reliable and valid for the stated purposes" (Nurrenbern & Robinson, 1994). I leave the larger part of this field to the social scientists; as a content-oriented researcher, I am more interested in 'instructional' variables than in 'intellectual' or 'psychosocial' variables. "Conclusions about the effectiveness of teaching techniques often are based on establishing significant differences between groups after the groups have been exposed to different educational experiences where these experiences are the independent variable" (o.c.).

My basic question, put in quantitative terms, could perhaps be: what is the relation between the structure and content of teaching (the educational experiences), and learning (significant differences in achievement)? What I would need then is some way to measure science proficiency. Now many educational researchers just take the scores on achievement tests and focus on what can be concluded with regard to the independent variable. They take the test itself more or less for granted. The researcher trusts that its validity and reliability have been assured and that the test measures what it is supposed to measure. It is necessary that science proficiency is measured unambiguously. Answers to questions on tests, questionnaires or interviews must be scored without any ambiguity and without any doubt with regard to validity. Here problems enter. First, there seem to be ways to pass such tests without understanding. Test preparation books contain interesting passages (Silver, 1993):

> When *we* teach you about Gibbs free energy we tell you exactly what you have to know to raise your CBAT [College Board Achievement Test] score. As we do that we drill you (in a friendly fashion) to make sure you're with us at every step. We'll show you, for instance, that you don't really have to *understand* anything about Gibbs free energy. You just have to 'know' that the symbol for Gibbs free energy is ΔG. If ΔG is negative, the reaction proceeds spontaneously in the forward direction. If it's positive, the reaction proceeds spontaneously in the reverse direction.
> You need to *associate*:
> NEGATIVE ΔG *with*: -reaction proceeds spontaneously in the forward direction.
> POSITIVE ΔG *with*: -reaction proceeds spontaneously in the reverse direction.
> When we get through with you, you may not really understand much about Gibbs free energy. But you don't have to, and we'll prove it. (...) You might not understand your answers, but ETS's [Educational Testing Service] scoring machine will think you do. ETS's scoring machine doesn't look for brilliant scientists, and it doesn't look for understanding. When it scores these two questions it wants to see D it the little oval spaces on your answer sheet. Stick with us, and you'll make the scoring machines very happy.

Fortunately, this nightmare is unlikely to unfold, since it is far from clear what exactly 'science proficiency' means with respect to organic synthesis, and tests do not abound. Parameters that could qualify, such as yield and purity, reproduction of textbook equations, or skilful manipulation, have already been criticized in chapter 2 for not being valid with respect to 'learning to experiment'. So instead of already having access to a set of data on science proficiency, this parameter still has to be clarified.

In the second place, even if this could be done, the parameter remains fundamentally ambiguous. To quantify, it is necessary that the meaning of all chemical terms is fixed and is the same for everybody. But this can only be achieved by acts of definition, which would deliver chemistry to the objectivist framework. The phenomenon of understanding would escape, which is unacceptable to me. I cannot take a set of standardized meanings to 'score' students' utterances; it is *their* meaning that interests me.

If it is acknowledged that students (and scientists!) can have different understanding of chemical words and statements and that these differences have to be taken into account, then students' answers are no longer compatible and can no longer be compared with the same tests and norms. *Consequently, the process in which students come to understand, that is, develop a viewpoint and move into a context, cannot itself be investigated in an objectivist way. Coming to understand is not a process that can be predicted and controlled because it is a process in history: understanding is a historic object and not an object for natural science.*

To put it differently, the problem is that quantitative techniques do not explain; they correlate. To establish a valid correlation, the independent variable (the teaching intervention) must be independent from the science proficiency measure. But in the hermeneutic framework this does not make sense. There is no way to talk about (let alone measure) understanding apart from the context of this understanding. So the meaning of the words used by students depends on the context in which the students acquired them. There is no way to establish science proficiency independent from the teaching context. This dependence does not have the character of a correlation, but of an explanation: the context gives meaning to students' words. Changes in the educational context (the independent variable) lead to *qualitative* changes in meaning, that is, students understand differently. It is therefore necessary to focus on the *process* in which understanding itself occurs and not on the *product*.

Thus, if research in science education wants to *understand* teaching and learning organic synthesis, a quantitative methodology is not adequate.

4.7 Conditions for an interpretive methodology

What, then, is it that would constitute a valid methodology for investigating understanding? In this section, I try to formulate the positive conditions for such a methodology. The first conditions concern the students and the teachers. Their understanding are issues for research, and the conditions specify the constraints that have to be met to investigate these issues. The last conditions deal with the understanding of the researcher. These explications of practical wisdom are enabling conditions for doing this kind of research.

Focusing on educational contexts

Studying understanding implies studying the contexts in which understanding occurs. Understanding as such can occur in many different settings, for example in daily life, in clinical interviews, through concept mapping, etc. But my aim is to study understanding as it occurs in relation to teaching. Hence, I should focus on educational contexts themselves.

Understanding as educational objective

In chapter 2 I described the cookbook problem and presented an analysis of the aspirin synthesis experiment. I found that, in cookbook experiments, understanding is not an issue. It can be concluded that not every educational process is equally suitable for studying understanding. It is possible to gather a lot of insightful information on cookbook experiments through observations and interpretations, but the phenomenon of understanding will not be illuminated. Consequently, educational contexts to be investigated must aim at understanding.

Chemical understanding

Another condition is that the kind of understanding I want to study must have a *chemical* nature. Chemistry as a science imposes norms on the quality of students' understanding. This quality is not related to general characteristics of understanding, nor with cognitive development. I must develop concepts that are more specific than 'problem solving capability' or 'maturation'. An implication is that the educational context must be able to represent chemistry as it occurs in 'real' chemical contexts. This is an effect of my viewpoint that knowledge and understanding are intrinsically linked to contexts. When I want to study how students learn organic synthesis, this means that they have to be engaged in an activity that can be called 'organic synthesis'. This poses a fundamental question: is it possible for educational processes to represent or simulate such contexts appropriately?

Learning as contextual development

I do not only want to study understanding, I also want to describe it as *learning*. Learning is achieving objectives. Students' understanding develops progressively: they apply prior knowledge and understanding in new situations; new situations thus should build on this prior knowledge and understanding. A methodology for studying students' developing understanding should thus have a longitudinal character. In hermeneutics, this can be seen as a progressive spiral of interpretation, understanding, and application, which can be described as *contextual development*. Learning in this respect is identical with scientific research, which also progressively moves through spirals of interpretation, understanding, and application.

To differentiate understanding from reproduction, it is important that the application is an action of the learner not pre-constrained by instruction. For example, when a topic such as acids and bases is taught through transfer of knowledge, in which concepts are defined and formulae derived by the instructor, and when this is trained by making pH-calculation exercises, then, after some time, a student might be able to perform such calculations correctly. However, I, as a researcher, would not be able to know whether the student understands acid and base chemistry, or merely applies algorithms. A sound methodology has to take this into account.

Learning in relation to teaching

Contextual development should not only be a result of understanding but it should also be linked to *teaching*. Learning can be independent of teaching: chemical researchers also learn while doing their work. Learning can also be unrelated to teaching, for example, when students are supposed to 'learn to experiment' whereas this objective is not explicitly advanced by the educational context. In such cases, learning depends on individual sense making efforts of the students. It thus is necessary that learning is explicitly linked to teaching. This implies that the constitution of the educational context also is an object of research. Educational contexts are constituted by the combined efforts of the designer of the educational material and of the teacher. Their understanding of the students' chemistry learning is constitutive for the students' understanding, and vice versa.

The object of research is constituted by the understanding of the researcher

The conditions mentioned above presume that the object for research already exists. This may or may not be the case. The quality of students' understanding is linked to the quality of the educational context. This last quality can be influenced by the researcher.

This feature is not accounted for by most interpretive methodologies. These only account for the fact that the researcher's understanding is influenced and shaped by the participants' understanding. In the case that interpretive educational research aims at understanding elements of social life in classrooms, laboratories, schools, and universities, there is much resemblance with interpretive sociology. The communal feature is that meaning is constructed through an interpretation of the social life of participants. A characteristic is that there are no given categories to interpret social life: the researcher has no privileged access to what is going on. Research is modelled after anthropology. However, I do have access to chemical contexts outside education. Thus, I can compare students' sense-making activities with my own knowledge and understanding of chemistry. A vocabulary is already given. But it is not inflexible. My understanding of chemistry is open to influences both from my efforts to understand how students understand chemistry, and from reflections on chemistry itself. My chemical understanding is normative with respect to students' understanding. I do not just have an impartial interest in students' understanding as it occurs in educational contexts; they should be prepared for doing chemistry. If students' understanding does not help them to do organic synthesis, this *must* lead to changes in the educational context. But it is up to me to judge this. I am in a position to change the 'social' environment of participants. Thus, students' understanding is directly related to my previous understanding of chemistry and to my understanding of the educational context. In this way, my understanding *constitutes* the object of my research.

The development of my understanding hopefully is progressive too. It can also have a cyclical element: I can turn my attention to the same educational contexts again and again. I can analyse the same material from different viewpoints; focus on different students, and try to probe deeper. I can develop new and more focused educational material on the same topic to test the adequacy of my understanding. Hence, there are cycles of interpretation, understanding, and application, with respect to my understanding of chemistry and of the educational context. This makes students' learning not just progressive from a rigid point of reference: they do not learn the same thing ever better, they learn it ever differently. The *quality* of their understanding is changed. In this respect, I do not primarily focus on individual students and their progress, but rather on my own progress. The methodology should provide opportunities for reformulating of research questions, for reflection on chemistry, and for developing new educational material.

I can only focus on what students do and say. These acts are governed by understanding. But understanding itself is in general not explicated: the focal point of verbalization is the issue, not the point of view that enables a verbalization. I cannot ask the students how they arrived at their point of view. The methodology must enable me to interpret students' acts in terms of points of view: to explicate which concepts govern students' understanding. The same holds for the teacher's understanding.

These preliminary reflections all seem to point in the same direction: to develop *new* educational material to study understanding, and to do this in a spiralling way. 'New', because existing material does not suffice, neither for learning nor for investigating; 'spiralling', because research questions develop during the process, and the answers to the question come in the form of interpretations, which, in a cyclical process, can be reapplied to test the adequacy of the researcher's understanding.

4.8 The cyclical method

Following the considerations mentioned above, a structure of research activities can be described. I refer to it as *the research cycle*, although it rather is *a spiralling* method. It is represented in figure 4.1.

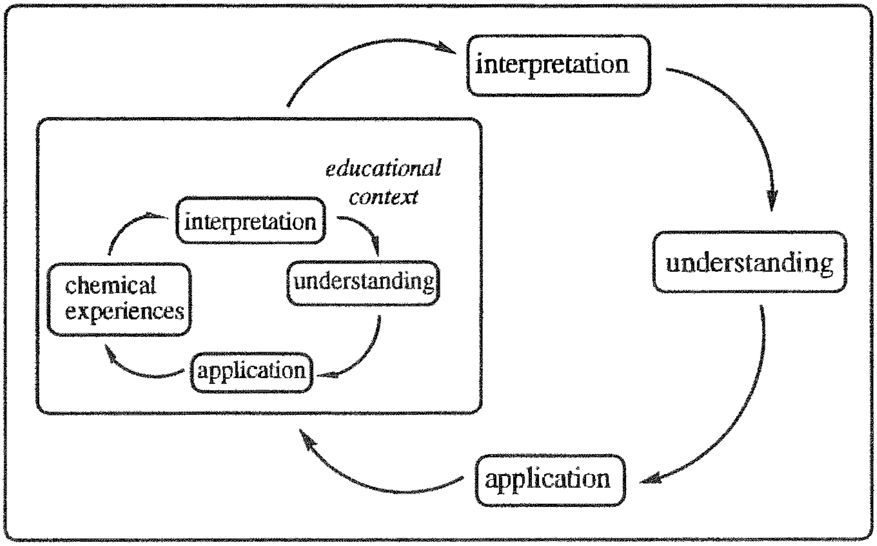

Figure 4.1 *The research cycle*

This method contains several cycles. Central is the educational context. The students' spiral is completely contained in this educational context. The students have to learn organic synthesis, therefore, they are in a chemical context in which they experience phenomena from chemical points of view. In this context, they act, observe, and interpret; come to an initial understanding; and apply this understanding to the chemical context in a second cycle. Since this happens in the context of education, the students activities can be influenced by the design of the educational context. The second (and the third, etc.) cycle can aim at a better understanding of the same chemical context, or move to a new, expanded context. This suggest a curricular structure of educational contexts–characterized by organic synthesis–that build on each other and also have an internal cyclical character.
The educational context contains the object of research: students' understanding. But this is a changing object, due to developing understanding of the researcher. This second

development has a similar spiralling character. The initial design of the educational context will largely be based on intuition, with only vague questions guiding interpretation. So although various things will be registered, there will not be a clear focus nor an understanding of one's own point of view. Interpretation will be guided by whatever question or issue emerges, to break through the hermeneutic circle. This will result in an initial understanding, resulting in educational issues coming into being. Some questions will probably be answered, but many more questions and inconsistencies will come forth. Hence, tentative explanations and hypotheses are formulated. These can be applied again by focusing on the educational context from a changed or new point of view and by developing different, supposedly better, educational material that enables the students to come to understanding. The researcher's cycle is twofold, since the understanding of chemistry changes as well as the understanding of the relation between teaching and learning.

The students' actions in the educational context are influenced by the teacher's actions as well as by the educational design. There are several options for including a teacher's cycle. If the researcher and the teacher are one and the same, the teacher/researcher will have some problems in registering the educational context, since it is difficult to observe and to teach at the same time. But these problems need not be fundamental and can be overcome with the help of audiovisual techniques. A more important consequence is that the students' understanding completely depends on one and the same person. It will be difficult to discriminate between the contribution of the teacher and the contribution of the educational context as designed by the researcher. In the case of teachers who are not the same person as the researcher, the teacher's understanding can be made an object of research, too. The teacher interprets, understands, and applies with regard to the students' developing understanding of chemistry. This process, combined with pre-service and/or in-service teacher education needs attention if the results of the study are ever to be implemented into a curriculum.

A last remark deals with the way I present this hermeneutic method in this study. It looks as if I figured it all out in advance, as if I first reflected on various theoretical frameworks and approaches to research, and then set down and discovered the research cycle. This in fact is a grotesque distortion of what really happened. The research cycle is itself a result of my developing understanding of doing educational research. It is with hindsight only that I can reconstruct what I apparently had been doing. However, I am unable to report on this historic process in a way that illuminates the development of this understanding itself. This is in part due to a lack of writing talent, but it is also due to the fact that I could not (and will never) find a place outside myself to observe from which point of view I myself am interpreting, understanding and applying.

4.9 Activities in the research cycle

The research cycle describes several phases that require specific methods and techniques. Interpretive research like this is not in all respects the same as interpretive research in the social sciences. I do not just investigate an unknown process, but I also influence the process to a great extend by developing the educational context. The adequacy of my interpretations is not only tested on new participants, but also in the act of constructing new educational material. Interpretive social researchers in general do not interfere in this way with the situation they want to understand, nor do they claim privileged excess to understanding. This implies that I should be careful in borrowing theories, models, and methods from social sciences like anthropology, sociology, and psychology, even if they share a commitment to interpretive research. Nevertheless, I have found several guidelines from such fields as interactionism and ethnomethodology very useful (Becker & Geer, 1960; Denzin, 1970; Erickson, 1986; Gallagher, 1991; Glaser, 1978; Glaser & Strauss, 1967; Guba, 1981; Maso & Smaling, 1990; Silverman, 1993; Strauss & Corbin, 1990; Wester, 1987).

Preparation for the research cycle

As always, research has to start somewhere, for instance with a reflection on the research objectives, leading to a set of initial questions. These have an unavoidable vagueness, since the researcher's understanding is not yet developed very well. In much quantitative social and chemical research, three questions should be answered before research starts: 'What is your question?'; 'What is your hypothesis?'; and 'What is your instrument?'. I could answer none of these questions at the outset. The words used in my initial questions and objectives, however, did not have much meaning. For example, an initial question was: 'How do students learn to do organic synthesis?' With hindsight, I can say that it was unclear to me then what I meant with 'learn to do synthesis'. However, it is anticipated that initial answers will lead to a reinterpretation and reformulating of the questions, making them more meaningful, too.

What I want to understand are the processes in which organic synthesis is taught and learned. Data should be gathered that disclose the moments of understanding of the students (and, if possible, the teacher). Their interpretation, understanding, and application must be disclosed in actions and discourse that take place in the educational contexts to be developed. Such educational contexts have to aim at chemical understanding.

I focus on organic synthesis experiments that are part of the first year laboratory course. In the first cycle, I turned to the existing curriculum and started research on the educational context present at hand. In a way, what I described in chapter 2 can be seen as a first revolution of the cycle. In the lab course, groups of eight students perform experiments under the guidance of a teaching assistant. The teacher's understanding is not a static object of research. The teacher is an intermediary between my understanding and the constitution of the educational context: the application of my understanding partly involves the teacher. So, the relation between my developing understanding and the teacher's developing understanding can be a research theme too.

It is the educational context that has to be interpreted. According to hermeneutics, this metaphorically means transforming the events into a 'text', in which phenomena, actions, and discourse can have a 'con'text. This is achieved with data gathering techniques. But what are 'data'?

It is impossible to register anything at all without a point of view. "The attempt to describe 'things as they are' is doomed to failure. Without *some* perspective or, at the very least, a set of animating questions, there is nothing to report. Contrary to crude empiricists, the facts *never* speak for themselves" (Silverman, 1993). The perspective I have is my wish to focus on understanding. It seems that I have to observe the educational context, with special attention to what the participants do and say. This implies that I can use those techniques that register actions and discourse: taking field notes, and making audio and/or video tapes. This material can serve to constitute the 'text' to be interpreted. But this will be meaningful only if the educational context explicitly aims at developing students' understanding.

Taking observation notes and video and/or tape recording implies knowing what to look for. Initially, this is far from clear. Fortunately, in a cyclical process, research questions and points of view can gradually develop. I started observing existing situations with only vague ideas on what to look for, but my vision gradually became more focused. The structure of the research cycle suggests to focus on the development of chemical understanding of the students; to focus on the influence of the teacher on this learning process; and to focus on the structure of the educational context as a whole in relation to the students' and the teacher's understanding.

Observation and interpretation

The aim is not just to produce 'thick' and 'authentic' texts on what is going on, but also to develop meaningful explanations. These explanations should be convincing, which implies that the observational data should be valid and reliable. "We cannot be satisfied merely with what I have called elsewhere 'telling convincing stories'. Contrary to the assumption of many social scientists, as well as funding bodies, generalisability need not be a problem in qualitative research" (Silverman, 1993). In order to convince the reader I follow several guidelines:

(1) *Comparison of different participants.* If understanding is related to structural elements of teaching, there must be something similar in different students' understanding. What is similar and what occurs again and again will be disclosed in comparing students who are otherwise in a similar educational context.

(2) *The principle of saturation.* That is, to continue collecting data only for as long as it can be expected that new things occur and new insights emerge. This principle to select a 'sample' is quite different from statistical principles. Groups need not be randomly selected, nor be sufficiently large to represent a population. The sample should cover all the qualitatively different activities that can occur in relation to a question or hypothesis. The quality of an action is related to understanding. Thus, if a quality is predicted and does occur, this cannot be explained as a random event. The word 'predict' should not be interpreted in an objectivist sense. 'Predicting a quality' means that something will occur that makes sense only from a specific viewpoint. The more specific a question is, the smaller the sample can be, since the focus is on a very specific element of understanding that can be easily recognized to be present or not. For example, if someone claims to be able to teach students a triple somersault in three hours, I will believe it if she or he can show me just one case.

(3) *Inspection of negative and deviant cases.* The focus should not only be on the exceptional student who shows brilliant understanding. It should also be explained why other students do not understand, or appear to understand things differently.

(4) *Focusing on what is observable,* (words, actions) and not on mental activity or on what people think they are doing. Categories such as motivation, attitude, cognitive ability, intelligence, etc., are not anathema, but they have to be derived from abstracted and generalized observations.

(5) *Providing observations as 'raw' as possible.* This implies, for example, making transcripts of tape-recorded discourse to allow the reader to differentiate between data and interpretation. I have made extensive use of tape recordings.
(6) *Formulating and testing qualitative hypotheses* (sometimes referred to as 'analytical induction' ((Fielding, 1988)). I am able to test hypotheses in two ways: by replicating with different groups to test whether the hypothesis has sufficient universality; and by using the hypothesis to develop new educational material and predict what will happen.
(7) *Researcher triangulation.* I have checked and discussed my interpretations with others, until agreement occurred. Such discussions are themselves a form of issuing discourse, in which new issues and points of view can be explicated.
(8) *Securing chemical validity.* The validity is secured by analyzing the chemical content of the educational contexts themselves and the students' understanding from the point of view of chemistry. The students' experiences should not only be 'authentic'; they should also prepare for doing research in organic synthesis.

Field notes, however complete and unbiased, are always the products of interpretation from a viewpoint. They cannot provide the amount of detail and the relative lack of bias that can be found in transcripts of recorded discourse. Heritage writes: "The use of recorded data is an essential corrective to the limitations of intuition and recollection. In enabling repeated and detailed examination of the events of interaction, the use of recordings extends the range and precision of the observations which can be made. It permits other researchers to have direct access to the data about which claims are being made, thus making analysis subject to detailed public scrutiny and helping to minimise the influence of personal preconceptions or analytical biases. Finally, it may be noted that because data are available in 'raw' form, they can be re-used in a variety of investigations and can be re-examined in the context of new findings" (Heritage, 1984), quoted in (Silverman, 1993).
During laboratory instruction, discourse takes place in two forms. Usually, there are meetings between teacher and students, in which elements of the experimental work (planning, theory, execution, results, etc.) can be discussed. Students and teacher also discuss things ad hoc at the bench. Both kinds of discourse provide valuable information, and both are 'naturally occurring', that is, unlike interviews or think-aloud (stimulated recall) protocols, they are part of the educational context itself.

I did not only *tape-record* discourse. In order to produce data as rich as possible, I interfered with discourse in two ways. In the first place, since I developed the educational material, I explicitly programmed group meetings to discuss the laboratory work. In the second place, I occasionally asked questions to the students, sometimes because I was curious, sometimes to make them formulate explicitly what they were doing and why, for the sake of the tape-recording. As a rule, I tried to refrain from giving directions or hinting at clues, in order not to distort the educational context. I acted like I thought a good teacher should act. Of course, this kind of *participant observation* does influence the process, but this is off-set by the gain in insight. I assume that the validity of the data is not reduced by my occasional participation in the process. The cyclical character of the research methodology allows to check this assumption by comparing the effects of interference with non-interference.

Making transcripts is not completely straightforward. People do not speak as if they read from a script. There is intonation, overlap, and silence, which all carry meaning. These elements point at things that remain unmentioned. Consequently, a transcript already interprets to some extent. I have focused on *what* is said (its *content* and *sequence*), because these seem to be related to the quality of understanding. I did not, for example, record the length of pauses, the loudness with which things are said, or specific emotions that could be detected, unless this seemed of particular influence to meaning.

I did not make extensive use of video recording. The disadvantage of video recordings is that it literally implies a point of view to take them, which influences the interpretation and hampers interpretation from different points of view. It is also much more difficult to transcribe a video recording than it is to transcribe tape recordings. I do not have a set of guidelines for doing this, and it would be a research project of its own standing to develop one. Moreover, making video recordings has a greater impact on students' behavior than tape recording and I simply did not have the resources to capture the laboratory activities of students fully with cameras.
I did make some video recordings, though. Uninterpreted video recordings could have added some value because they can be seen and interpreted again and again, leading to new insights. However, I found that they added little to my observation notes. I think this is because I focus on understanding, and not on manipulative skills. The medium of understanding, according to hermeneutics, is language. If applications are meaningful, it is possible to describe and talk about them meaningfully in words, even when this is vague or incomplete. For this, I can rely on my observation notes. The language to describe meaningful actions is partly provided by the participants, whose understanding is disclosed in their way of saying things, and partly by my observations, which are expressed in the notes.

The data are analyzed from the point of view of the questions to be answered. The basic assumption is that the data (for example, students' actions and assertions) make sense, because if we want to understand others, we must assume that they are sensible human beings who are right from their point of view. Davidson calls this the Principle of Charity (Davidson, 1984, p. 27): "Charity in interpreting the words and thoughts of others is unavoidable (..): just as we must maximize agreement, or risk not making sense of what the alien is talking about, so we must maximize the self-consistency we attribute to him, on pain of not understanding *him*". Students are not judged from a fixed point of view supposed to correspond with what is chemically correct. The question is not whether what students do or say is right or wrong, but whether it makes sense from their point of view. To arrive at a consistent interpretation, it may be necessary to revise the points of view from which my questions were posed. Since students may interpret chemical phenomena quite differently from what is expected and may do and say strange things, this should issue a reflection on chemistry on the part of the researcher. I, as a chemist, use my chemical knowledge to form expectations on what is sensible to do in a certain chemical context. Since students may act differently (but rationally), I have to rethink my chemical understanding to find out what it is in chemical issues that enables students to see these as they do. This reflection can influence my own understanding considerably. The meaning of chemical concepts changes and develops. Thus, I also learn chemistry, and reapply these deeper insights in my analyses and educational material. This is not common in educational research, which often does not reflect at all on the meaning of chemical concepts, but instead borrows them wholesale from experts or textbooks or memory.

Valuable data also come from the writings of students: their lab notes and reports. These can reflect the results of their understanding. Sometimes these texts give additional information on topics that for some reason never entered discourse. Sometimes they are essential to interpret students statements, especially when they refer to such things as spectra or other chemical data.
Other texts that can be analyzed are the texts used in education. These texts are meant to structure the activities of teacher and students, and consequently are part of the context of understanding. For a part, the texts are made by myself. This allowed me in a way to do research on myself, for example, when I ask myself the question what I intended to achieve with a certain assignment. The educational texts, like the field notes and interpretations, can be used to analyze my own developing understanding. Other texts are those used for reflection: textbooks, lab manuals, primary sources, and texts stating curriculum contents and objectives.

Understanding and application

It is quite likely that it is not possible to give a definite and unambiguous answer to the research questions. This may be due to elements of the educational context. Certain tasks or questions may lead students in an inproductive direction, or texts or teachers may give away crucial information distorting students' actions and interpretations.
From interpretation, these issues can be understood. Questions are answered, viewpoints revealed, relations formulated, problems detected, or not. In this process, understanding occurs. As a consequence, new and more specific research questions can emerge. Some of these can have the character of hypotheses. If it is true that students make sense of chemical phenomena by applying specific concepts, then it is possible to predict qualitatively what they will do. Of course, 'hypothesis' and 'prediction' are not meant in any objectivist sense. It is not the exact sentences or actions that can be predicted but the way of making sense.

On the basis of the interpretations and reflections, new educational material can be constructed that allows for answering the new and more specific questions and for investigating hypotheses. A new educational context is constituted, and a new cycle of the spiral can start.
In a first cycle, it cannot not yet be very clear which criteria should be used to develop this new material. The material may be based on intuitions, on suggestions from staff, teachers, and/or students, and on standards of logic and consistency, but not yet on empirical results. This may change when sequences of data have been produced, revealing how teaching and learning are related with regard to this specific area of chemistry. This will provide research based criteria for the reconstruction of the material in subsequent cycles. Registration of meaningful events in the educational context can become increasingly focused, because the educational context is increasingly based on an application of interpretations of previous registrations. The application is an essential companion to understanding. The application makes understanding explicit, and discloses the quality of understanding.

The new material will still be constrained by various existing conditions that cannot be offset. These can include timetables, the experience of the teacher, the students' prior knowledge, the opportunity to teach teachers, the availability of apparatus, the permission to deviate from the official curriculum, and so on. Research may suggest significant changes, and this may sometimes result in a conflict with existing opinions.
I focus especially on understanding the educational process. An objective that is closely related is improving the quality of education by applying the results in curriculum reform. From this point of view, the development of new educational material should aim at optimizing the material. From the point of view of the more theoretically interested researcher, the new material should allow for new research questions to be answered. These points of view need not contradict each other, but they may.

The results reflect the researcher's understanding. Results can be interpretations and hypotheses on students' understanding; descriptions of the development of chemical meaning in educational contexts; and new educational material that is consistent with this contextual development. From the point of view of formal research, this new material can be regarded as spin-off. From the point of view of curriculum development, it can be seen as the main result.

5 Interpretation

5.1 An introduction to the empirical chapters

In this chapter, I start presenting the empirical results. I have developed and investigated several educational contexts, each new one applying the understanding that resulted from interpreting the previous one.
To describe this process, I had to solve a hermeneutic circle problem. The results and the educational contexts are self-referential: one can only understand the meaning of the results in terms of the educational contexts, but the educational contexts have been developed by applying the results. They give each other meaning, which makes it difficult to describe the one without simultaneously describing the other. In other words, my activities are based on my understanding, whereas my understanding is based on my activities.
To solve this problem, I start this chapter with a description of the issues I eventually applied to interpret the educational contexts. These issues can be seen as the final results of my research. Presenting them right away is, I admit, a blunt form of transfer of knowledge. Fully describing the genesis of the issues, with all its detours and dead allies, would not fit the format of this study, which, after all, is not a textbook to be used in education. I expect the reader to understand enough of the context to be able to follow my presentation. I will nevertheless attempt to convince the reader of the truth of the issues by regularly describing instances that led to their disclosure and development.

After presenting the issues I apply them to describe and interpret the first new educational context I designed. In this context, which I will refer to as *Esters 1*, students investigate processes of making esters. This first new educational context is a convenient starting point because it is a first attempt to develop an alternative for prescription experiments, and as such it can be understood from the analyses presented in chapter 2. I will thus describe my original intentions and expectations, to show that the final issues played only a marginal role in this stage of research. I then present and interpret data on how students acted in Esters 1. In the presentation of this I try to show how the issues emerged. My improved understanding I then applied to revise the educational context. This led to a second cycle and a second educational context, Esters 2. In the same spirit, Esters 3 and Esters 4 came into being. I describe the research on these contexts in the next chapter. The understanding resulting from the interpretation of Esters was also applied to expand the educational context of organic synthesis. This new context is called *Ethers*, because the phenomena students experience and the issues they have to focus their attention on are situated in the synthesis of ethers. I describe this in chapter 7.

The students were always informed in advance by letter about the research taking place. Their permission was asked for observation, recording, and use of data made anonymous. All students always granted their permission.
In this chapter and in the next few, I will make abundant use of transcripts: fragments of (tape) recorded and transcribed discourse. These transcripts are in Dutch and are available for interested readers at the Department of Chemical Education of Utrecht University (Van Keulen, 1995). I have translated the parts I use into English, trying to preserve the

meaning of what is said. This sometimes was difficult since occasionally sentences were spoken that were grammatically incorrect or lacked clear meaning. In such cases, the translation tries to preserve the ambiguity and imprecision of the original. In this chapter, all references are from the transcripts of Esters 1. The students are indicated with a combination of a letter and a number. The letters are in chronological order of my research: a and b belong to Esters 1, since Esters 1 was carried out twice with two groups of eight students. C and d belong to Esters 2; e, f, g and h to Ethers 1; etc. All teaching assistant are indicated simply with 'TA', since all groups had different TA's and did not interact. I myself am indicated with R.

5.2 The research cycle and the teacher

Hermeneutically, the teacher's activities should be based on an understanding of the students' cycle. Teachers sometimes have two roles: they design the educational material and they also teach it. In my research situation, the teacher and the designer are not one and the same person. I design, others teach. Ideally, the teacher's understanding is a result of an understanding of what happens in the students' cycle. Like students who have to learn chemistry in a chemical context, teachers have to learn in the context of teaching. Consequently, the teacher's understanding and research on the teacher's understanding is one cycle behind on research on the students' understanding.

However, research on the teacher will be almost absent in the empirical chapters. The reason is that, under the practical conditions of my study, it was impossible to investigate the development of teachers' understanding. Usually, teaching assistants at M&M1 stay on the course for a very limited time. The typical teaching assistant is a student or young research chemist with little or no teaching experience fulfilling his or her teaching obligations at this lab course. It is common practice to teach the course (or even half the course) only once; this often implies that a TA teaches an experiment only once. The TA's have some time to prepare for the experiments, but this barely suffices to get acquainted with all the theoretical aspects, the equipment and the actual conduction of an experiment. A typical preparation involves reading the student and teacher manuals and doing those parts of the experimental work with which the TA is unacquainted.

This situation is recognized by the director of the course as far from perfect. He tries to make the best of it by making the experiments 'teacher-proof', that is, to select experiments that have a high chance of chemical success, and to provide students and teaching assistants with manuals that cover every detail of the experiment, to prevent chemical and organizational problems[1].

According to the cyclical approach, a TA would prepare for an experiment, teach it, and reflect on what happened. He or she would interpret the teaching experiences, come to an improved understanding, and apply this in the next cycle. However, there is no next cycle. Consequently, there is no incentive for TA's to interpret the educational context. And, I cannot investigate a teacher's cycle.

The TA's participating in this study (volunteers, not chosen by me) did not deviate from the average. In general, they had no teaching experience whatsoever. Chemically, they of course were more experienced than the first year students, but they seldom had any research experience within the field of organic synthesis. This of course influenced their

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[1] J.L. Derissen (director of M&M1), private communication.

ability to teach in a context of preparing students for doing research in this area: they could not build on their own understanding of teaching and of research in organic synthesis. This implied that they relied heavily on the preliminary teacher training. The facilities for this, however, were more or less the same as for other, traditional experiments.

I also wrote a teacher manual for each version of my experiments, in which I tried to explain the experiment and my intentions. The manual describes my expectations regarding students actions and interpretations. I indicated the kind of experiences the students could have when they executed the tasks. I also indicated possible questions to probe students knowledge and understanding, to draw attention to relevant experiences and observations, and to help students to explicate and conjecture.

The teaching assistants were prepared for the experiments under my guidance. I tried to reinforce my intentions by 'lecturing' to them. My hope was that when they would experience similar phenomena as the students were to, this would help them to supervise. However, since I also had to transfer to them my interpretations of the experiences, their experiences could never be the same as those of the students. The TA's knew the 'correct' answers to everything. They for instance smelled 'esters', whereas the students smelled 'something sweet'. In this way, I provided the TA's with information and not with understanding. I gave them a paper prescription on what to do, a recipe so to say. But within the given constraints (no second cycle, no time for rigorous preparation) I saw no alternative.

Although the teaching assistants co-operated as best as they could, it was not to be expected that they could reach optimum results in just one cycle. Nor did they (or the students) profit much from the teaching experience they acquired, since almost never did a teaching assistant supervise an experiment twice.

The only research-based development regarding the teacher's cycle is to be found in my revisions of the manuals. I was able to predict more accurately the range of activities that students would engage in; the chemical results of these activities; and the interpretations that the students would give of their experiences. In this way, the TA's were probably also better prepared for what would happen, but, more important, the student manual provided the student with a better structure for learning.

My imperfect solution to this teacher problem has been to interact occasionally with the teaching process. As a researcher, I was always present during the conduction of the experiments. I invariably started with giving a brief introduction of myself as researcher. I sometimes interfered by asking additional questions to students, or returning to issues the TA skipped. In this, I tried to do those things the teacher paragon I had in mind would do. I never was a mute observer; I often asked questioned the students on what they were doing. This sometimes interfered with what otherwise could have happened. The TA's were not always confident about what they were doing. I often had short discussions with the TA's to give them advice. Sometimes the students turned to me for advice. In such situations, I tried to behave as I thought a teacher in this educational context ought to. That is, I tried to avoid giving direct instructions to do this or that; I refrained from using words like 'good' or 'correct'. I assumed that I did not know what would happen, and that it was the students' responsibility to find out what was going on. During group discussions, I sometimes asked additional questions because I wanted the students to explicate their experiences and interpretations.

By taking this role, I made it impossible to study a teacher's cycle. But this was no possibility anyway. I gave priority to gaining a better insight in the students' understanding.

5.3 The issues

In this section I describe the issues that, I think, determine the meaning of an educational context that prepares students for doing research in organic synthesis.

Synthesis-planning

The issue of *synthesis-planning* was first constituted by De Jager (De Jager, 1985). He discovered that students, when carrying out prescribed syntheses, recognize that there are separate stages (formation, purification, and characterization) in all procedures. They used the intervals between the stages to have a coffee break. However, they did not see relations between these stages, although almost all successful synthesis procedures contain choices that can be understood only from the point of view of another stage. In chapter 2 I described the synthesis of aspirin, which is a beautiful example of careful synthesis planning from a chemical point of view. For instance, an excess acetic anhydride is used because it is easier to remove this excess than to remove left-over traces of salicylic acid in the subsequent purification stage.

It seems that if students are to learn to do organic synthesis they should learn to recognize such relations. I applied this synthesis-planning theory already in the first version of Esters. In this educational context, students are making certain esters from carboxylic acids and alcohols. They have to come to an understanding that the stages of formation and purification are linked: when they start the ester synthesis with equimolecular amounts of starting reagents it is much more difficult to purify the product than when they use an excess of carboxylic acid.

Reaction-type

I designed Esters 1 explicitly to enable students to understand synthesis-planning. The chosen reactions constitute an equilibrium in which a considerable amount of starting reagents will still be present. I expected students to know *and understand* equilibrium. I expected that, when they would find that the reaction mixture still contained starting reagents after reaction, they would realize that they were dealing with a reaction proceeding towards equilibrium. When interpreting the data on Esters 1, I concluded that students were not exactly looking at things that way. Although most students knew that esterification reactions are equilibrium reactions, they did not apply this knowledge to interpret their experiences. They appeared to have knowledge without understanding. Many students also ignored the formation of water as a by-product. They did not expect the crude reaction mixture to contain anything but the ester. The word 'synthesis' seemed to suggest to them that the reaction proceeds towards complete conversion into the product. Schematically, the students based their actions on a reaction-type conception of the type $A+B \rightarrow C$, instead of on the type $A+B \rightleftarrows C+D$. The prototypical *reaction-type* $A+B \rightarrow C$ represents several issues. It represents a stoichiometry: one mole A reacts with one mole B; it represents completion: when the reaction is finished all reagents have been transformed into the product; it represents the absence of attention to by-products; and it

represents the absence of attention for the analysis of a *mass balance*, which would enable a conscious interpretation of the reaction-type under consideration.
Determining the mass balance means determining the composition of a given mixture in terms of the *identity* and relative *quantity* of all the substances present. Thus, an understanding of the issue of reaction-type as such means the ability to focus on the parameters identity and quantity in a mass balance. An understanding of specific reaction-types allows for drawing specific conclusions.
In a reaction that comes to *completion*, only one identity (C) is present, in a 100% quantity. When a *by-product* is formed, the crude mixture contains different identities (C+D). Relative to the starting reagents, a 100% quantity of both C and D still is possible, therefore, there is no need to have attention to the issue of quantity itself. In *equilibrium* reactions it becomes necessary to make quantity into an explicit issue. The crude mixture contains several identities (A+B+C+D) in quantities that are related to each other through an expression known as the concentration quotient. This introduces specific ways of manipulating the relative amounts, namely by using an excess amount of one of the reagents or by removing one of the products. In a *side-reaction*, the different identities and relative quantities are not related to each other through one formula. Manipulation of relative quantities is often possible through changing the reaction conditions, but changing the relative amounts of the starting reagents does not produce predictable effects. Another possible reaction-type is that the product reacts again with one of reagents: a *subsequent* reaction.

In a prototypical reaction-type concept, students pay no attention to identity or quantity; they simply expect the reagents to be completely transformed into the product. With such a conception in mind, it is unlikely that the students will plan any synthesis procedure successfully. It seemed necessary to develop an understanding of the issue of reaction-type. This became a major influence on the design and interpretation of educational contexts after Esters 1. Table 5.1 comprises the reaction-types mentioned.

Table 5.1 *Some reaction-types*

$A + B \rightarrow C$	The prototypical reaction-type
$A + B \rightarrow C\ (+ A + B)$	Reaction practically coming to completion
$A + B \rightarrow C + D$	Formation of a by-product: identity becomes an issue
$A + B \rightleftarrows C\ (+ D)$	Equilibrium: the reaction mixture contains both product(s) and starting reagents in a certain quantitative relation: quantity becomes an issue
$A + B \rightarrow C + D$ $A + B \rightarrow E + F$	The side-reaction: the same starting reagents can react towards different sets of products
$A + B \rightarrow C$ $C + A \rightarrow G$	The subsequent reaction: the product reacts again with a starting reagent

It would of course be very easy to tell students directly that some reactions proceed almost to completion, whereas others form an equilibrium mixture, etc. However, my aim is to develop an *understanding* of these reaction-types. Understanding underlies the capacity to apply in appropriate contexts. Direct transfer of information does not lead to such a productive understanding.

Structure-activity-relations

De Jager worked from the presupposition that students are unable to design the formation stage with respect to reactants and products. In his design-oriented experiments the reactants were selected in advance. In Esters 1 I took the same attitude. The reactants–alcohols and carboxylic acids–were chosen by me, without planning to focus explicitly on the question why an alcohol reacts with a carboxylic acid to form an ester. However, the students appeared to be very much interested in such questions. I realized that the question why a given substance reacts with another to form a specific product lies at the heart of scientific synthesis and of organic theory.

In contemporary organic chemistry, reaction potentiality is related to the molecular structure of substances, especially to functional groups. The knowledge that certain substances can react with carboxylic acids towards esters is represented in the molecular structure by the presence of an OH-group. Students know the positions of atoms in a variety of molecules because this is adequately represented by most representations such as molecular formulae and ball-and-stick and space-filling models. But these models do not represent the chemical reaction potentialities themselves, nor the mechanisms through which atoms exchange position. For organic chemists at the last decade of the twentieth century, accustomed to such techniques as infrared, NMR, and GC-MS, it has become routine to equate a substance with its molecular formula. Students of chemistry appear to have the same attitude. When you ask, 'What is an alcohol?', they immediately reply with a molecular formula featuring an OH-group. However, on interpreting my data, it seemed to me that, to students, this often is little more than a label. They do not imagine or understand the range of reactions possible with this group. They see the OH-group as a *characteristic* group of certain molecules, and not so much as a *functional* group of certain substances. In other words, they only possess information on atomic positions and not an understanding of the chemical activity that is represented in this way.

Organic synthesis is a way to improve understanding of chemical activity. The models are made of mechanical objects, which seems to suggest that synthesis is screwing and unscrewing atoms. It is not. Organic mechanisms are not purely mechanical. A successful synthesis can be proof of certain non-mechanical parameters influencing the chemical behavior of the substances. Such parameters are tacitly represented by the models if specific units can be understood in their functionality. This *structure-activity-relation* is the third issue that came to influence my designs and interpretations. 'Structure' represents those chemical phenomena ('activities') that are already understood; it can be applied to describe new phenomena.

Since there is a *chemical* relation between the macroscopic behavior of substances and molecular structure this implies that it is possible to deduce structure-activity-relations from macroscopic phenomena. This was already well understood in the nineteenth century: functional groups were established long before the atomic hypothesis was accepted. I do not propose to repeat history in education; I propose to design a *hermeneutical* road that starts with experiences with substances and reactions and proceeds to an understanding of functional groups and structure. This in contrast with the objectivist way of presenting students with information on chemical structure. The results of the historic processes in which chemists have objectified their experiences may be communicated effectively to students by way of transfer of information, but it is not a successful way to prepare students for understanding.

Simulation-of-research

The way to unify the issues mentioned above is to incorporate them in what I eventually came to mention *simulation-of-research*. This issue, however, was not an issue for me when I started. Instead, I used the concept 'open'. Esters 1 was designed not to be a prescription experiment but to be an open, design-oriented experiment. A prescription experiment is 'closed', because the question, the methods, and the answer are known in advance. I wanted to give the students freedom to choose methods and answers, by giving them the question 'How can we make esters?' I had expected that such a question would become the leading question for the students, and that they would derive their actions from a reflection on their experiences from the viewpoint of this question.

In this, I was disappointed. In the first place, I noticed that students very often asked their TA, 'What do we have to do now?', instead of deciding by themselves. The question I posed did not seem to become their question so easily. In the second place, on a hidden plane, Esters 1 was not open at all. I really wanted the students to make esters, which meant that the answer was fixed in advance, after all. This implied that certain methods were predetermined, too. Students would arrive at pure esters only if they employed certain methods. I did not prescribe those methods, but I inserted some tricks that, in my mind, would allow students to deduce the 'right' methods and answers. At least, that is my present taxation of what I did. In my first designs I felt unsure whether students would experience the phenomena I considered important. And even if they would, I was unsure whether they would interpret the phenomena from my point of view. There was no guarantee that students would do the things that would help them to solve the synthesis problems. I tried to make sure that students would at least get the 'right' experiences. A closer look at the text of the student manual (which will be discussed in the next section) reveals that I had failed to create a context in which students could move ahead by themselves. Like cookbook experiments, Esters 1 had several prescribed assignments. For instance, students had to do test tube experiments and infrared and refraction index measurements. I expected that students would know that esterification reactions are equilibrium reactions. But I was not sure whether students would apply this knowledge by using an excess amount of acetic acid in the formation stage. That would mean that they would experience problems with purification without experiencing an appropriate clue. Thus, I instructed the TA to assign one of the duos the task to carry out the reaction with an excess amount of acetic acid. These students would be able to purify their product, since it would contain hardly any alcohol. I expected that, after comparing the final purification results with the other students in their group, everyone would understand the superiority of a formation stage that takes into account purification problems.

It is clear that there is a tension between professing that students take decisions themselves and instructing them to do things they would never do themselves. The difference with cookbook experiments is that in a cookbook experiment the prescriptions lead to a synthesis product, whereas in this educational context the prescriptions lead to experiences to be applied in the decision making process. However, it did not always work. For instance, students mixed water with butyl acetate, just as they were assigned to do, they noticed that these liquids do not dissolve in each other, they wrote this down and then they felt they had completed the task. But it did not dawn on them that they were supposed to apply this experience the next day by using water to get rid of unreacted acetic acid from the crude reaction mixture of butyl acetate. The activities lacked meaning.

Not only did several instructions fail to achieve their goal, they also stand in conflict with what happens in chemical research, where nobody stands beside the bench and whispers what to do next. The relevance of phenomena can only be understood from a chosen point of view. Students executing *tasks* do not have a point of view. They do what they are told to do. I understood that I should drop such tasks and instead focus on developing questions and viewpoints. Students should ask themselves how to make esters, how to purify them, how to find out whether purification was successful, etc. This issue, which I called *simulation-of-research*, also influenced the educational contexts considerably. *The phrase 'simulation-of-research' seems appropriate since problems, questions, and conjectures have to guide students' actions, like it is in research.* Although I was at first reluctant to drop specific instructions, afraid that students would otherwise never find clues for resolving their synthesis problems, I found the results rewarding.
Simulation-of-research thus became a tool for constructing the educational context, and a tool for the teacher to create the appropriate atmosphere. From the students' point of view, it leads to an integration of the three other issues within the context of doing research. The student has to learn to do research, not just to learn to design a prescription for making organic substances. The initial question on how to make esters leads to an awareness of the purification problem. This necessitates a careful analysis of reaction mixtures to establish a reaction-type. The reaction-type (equilibrium) demands a rationale, which is to be found in structure-activity-relations. In this way, synthesis is part of organic chemical research, which seeks to understand and predict the properties of substances. In this way, the educational context may help prepare students for doing research.
To achieve this, the educational context has to be modelled after the hermeneutical cycle. A phenomenon will only become an *issue* for the students if they develop explicit attention. Such an attention results from reflection on and interpretation of experiences. Cutting corners by offering clues before something has become an issue does not work.

These four chemical education issues play a role in all three hermeneutic cycles. The students have to develop an understanding of these issues to be able to do organic synthesis. This student-understanding may remain tacit to them. On the explicit level, students make esters, build reflux apparatus, analyze samples, etc. This is what they talk about. But the ability to act and talk successfully depends upon an underlying understanding of the issues. The TA has to have a more explicit understanding of the issues, since she or he has to create a learning environment in which students can come to an understanding. This should be done purposefully instead of intuitively. The researcher, finally, has to disclose and explicate the issues; to establish them as being fundamental to organic synthesis; and to apply them in designing appropriate educational contexts.

5.4 The first version of Esters

I will now describe the first version of Esters. The leading idea in this educational context was the wish to achieve an understanding of an element of *synthesis-planning* without making use of knowledge transfer. The element of synthesis-planning I had in mind is that students should learn to take into account possible purification problems when designing the formation. The purification problem is the difficulty of separating the product ester from the starting reagent alcohol. The origin of this problem lies in the fact that the esterification reaction proceeds towards an equilibrium instead of coming to

completion. A solution for this problem is to use an excess amount of carboxylic acid during formation. I tried to get students in a position from which they would develop this solution themselves, on the basis of their own experiences.
In this section, I present the whole text of the student manual. I will do this in fragments that correspond with stages in the experiment. Each fragment will be commented upon to disclose my intentions and expectations at that time. I will occasionally criticize my text from the viewpoint of my later understanding. The original text is in Dutch. What follows is my translation.

> ### 1. Introduction
>
> In this experiment you are going to make a few compounds that are called 'esters'. The word chemists often use instead of 'to make' is 'to synthesize'. The intention of this experiment is that you start with learning synthesis. In a way, it is an 'experimental' experiment, that is, research is being done to determine the best way to treat this subject. This implies that, apart from your teaching assistant, you will encounter a researcher. Through observation, he tries to investigate how students learn to synthesize.
> The researcher will have no influence whatsoever upon the assessment. The research data will be made anonymous and will not be available to others except the researcher.
> It is not necessary to prepare for this experiment. During the prelab discussion the teaching assistant will inform you about what will be done.
>
> ### 2. Contents
>
> The experiment consists of the following parts:
> 1. Prelab discussion
> 2. Test tube experiments
> 3. Second group discussion
> 4. Refluxing
> 5. Assignments

On the basis of the secondary school curriculum, I assumed that the students would know the names and general formula of esters, and that they would also know that esters can be made from carboxylic acid and alcohol. Perhaps they even would know that esterification reactions proceed to equilibrium. These assumptions are checked and discussed in the first, prelab, group discussion at the start of the experiment. This discussion revolves around the question 'How would you make an ester?' The teaching assistant is supposed not to give away crucial chemical information but instead to listen carefully to students' ideas and suggestions, and to give opportunity for these ideas to be executed. The characteristic sweet smell of many esters is made an issue by showing jars containing pure esters and allowing students to smell. I expected that students would answer the question by suggesting to put together an alcohol and a carboxylic acid.

> ### Test tube experiments
>
> In this part you will get acquainted with the substances and the reaction on a test tube scale. This is a preparation for the next part, in which you will be performing two reactions on a larger scale.
>
> **Assignment 1**
> Determine from a book on laboratory safety the hazards associated with: concentrated sulfuric acid, 1-butanol, formic acid and ethyl acetate. Write down in your lab note book what you should do in case of an accident. Take the necessary preparations.

Assignment 2

Make in (marked) test tubes the following reaction mixtures:

a) 1 ml methanol plus 1 ml acetic acid
b) 1 ml ethanol plus 1 ml acetic acid
c) 1 ml 1-butanol plus 1 ml acetic acid
d) 1 ml 1-butanol plus 1 ml formic acid

Let these mixtures rest for a while and write down your observations.
After that, add, using a Pasteur pipette, 10 drops (or: a little dash) of concentrated sulfuric acid to each test tube. Shake each tube.
Again, write down your observations.
Fill a test tube with 1 ml of formic acid and add a dash (10 drops) of sulfuric acid.
Write down your observations.

The assignment on safety precautions is typical for M&M1. Every experiment is supposed to pay attention to this issue in this way.
In the second part called 'test tube experiments', the students have to make mixtures of formic acid/acetic acid with methanol/ethanol/1-butanol. It is expected that this activity is in accordance with students' statements from the prelab group discussion.
Not much will happen within the first few minutes after mixing, since the esterification reaction is quite slow. After several minutes, a faint sweet smell becomes noticeable in the test tube containing formic acid and butanol. It takes considerable time for other combinations to develop such a smell. After writing down their own observations, the students have to add sulfuric acid. This substance catalyzes these specific reactions and will thus speed up the reaction rate. I did not expect students to come up with this idea themselves. Therefore, I programmed it to create the experience. In this way I planned to draw attention to an element of synthesis. I hoped that students would realize that mixing the appropriate reagents is not always sufficient for formation. The formation can be influenced, for example with a catalyst.
The catalyzed reaction leads to a swift development of a sweet smell. The only thing to be seen will be the development of small gas bubbles in the combination with formic acid, due to oxidation of formic acid in the presence of sulfuric acid. Thus, sulfuric acid should better not be used to catalyze esterifications involving formic acid. In a last test tube experiment, I tried to make this an issue by having students directly mix concentrated sulfuric acid and formic acid, to draw students' attention to this problem.
Since all reactants and products are colorless liquids, it is rather difficult to *see* anything happen. This focuses the students' attention to the important issue of characterization as a part of synthesis. These esterification reactions produce esters that have a characteristic smell. The development of this smell thus is a measure of the reaction taking place. But it is a very subjective and crude measure, making students realize that a better technique should be chosen.

In the upcoming discussion the following questions will be raised:
What are your observations?
What did you expect to see?
Which conclusions do you draw from you observations?
Are you satisfied with the result? Why/why not?
What would you have to do to obtain the ester?
Try to formulate answers to this.

After these experiments a second group discussion is planned in which the observations, results, and conclusions with regard to the test tube experiments are discussed. It is expected that students will be disappointed by the results of the test tube reactions: not much seems to happen, unless sulfuric acid is added. Even then things are not very clear. Students are brought in an issuing discourse. They all have their own, immediate experiences. Consequently, each student will defend her or his interpretation. It will be felt that, to reach agreement, some sort of explicit consensus is necessary to come to grips with what is going on. I was hoping that in this discourse some issues would emerge, but I had no idea what exactly would happen. Eventually, interpretation of students' discourse led to the issue of structure-activity-relations. Although simulation-of-research had not yet become an explicit issue at that time, it is foreshadowed in this part of the educational context, because students are brought in a position to formulate points of view from which experimental hypotheses can be deduced.

I anticipated that students would propose to carry out the larger scale versions of the reaction at elevated temperatures and in the presence of sulfuric acid. Since students are unfamiliar with lab equipment, the TA would introduce them to the refluxing technique, which, I thought, they will be able to understand.

I wanted to test whether students are able to use synthesis-planning in advance. Theoretically, they are not supposed to understand this issue, since they lack experiences in an appropriate context. That is, presenting students with all the appropriate information does not lead to application. I had the TA tell the students that these reactions, like many other esterification reactions, are equilibrium reactions, with an equilibrium constant K of about 4. I also gave them a table including boiling points and solubilities of the substances. From this table it can be deduced that it is difficult to separate ester and alcohol. I expected that students would not use this information when choosing relative amounts for the formation stage to prevent separation problems.

Refluxing

In this part you conduct two syntheses in a so-called reflux apparatus. You can read about this technique in the laboratory manual of M&M 1 in the chapter called 'Apparatus'.
The table below gives some properties of the substances to be used.

Table 1: Properties of the substances

substance	M (g/mol)	Boiling point (°C)	Density (g/ml)	Refraction index
water	18.0	100.0	1.0	1.3330
sulfuric acid	98.1	338	1.8	1.405
acetic acid	60.1	117.9	1.05	1.3716
formic acid	46.0	100.7	1.2	1.3714
methanol	32.0	65	0.79	1.3288
ethanol	46.1	78.5	0.79	1.3611
1-butanol	74.1	117.2	0.81	1.3993
methyl acetate	74.1	57	0.93	1.3595
ethyl acetate	88.1	77.1	0.90	1.3723
butyl acetate	116.2	126.5	0.88	1.3941
butyl formiate	102.1	106.8	0.89	1.3912

> Each duo will conduct two different syntheses, of a total of eight variants:
>
> 1: methanol and acetic acid
> 2: ethanol and acetic acid
> 3 and 4: butanol and acetic acid in two different ways
> 5: butanol and acetic acid
> 6: butanol and formic acid
> 7: ethanol and acetic acid
> 8: ethanol and acetic anhydride
>
> The teaching assistant distributes the variants between the duos and will give additional information.
> Conduct the reactions with 30 ml of acetic acid (or formic acid)
> Determine yourself the amount of alcohol needed, using the data from the table.
> Your TA will help you building the apparatus and will determine when you are allowed to start refluxing.
> Reflux the mixture for at least one hour.
> During refluxing you work on the following tasks.

In a group of eight students, each duo would carry out two syntheses, chosen from predetermined combinations. So there will be eight slightly different versions. This will enable students to compare their results, learn from each others experiences, and come to consensus.

The 8 variants are not all different. Variant 4 and 5 are the same, as are variants 2 and 7, unless the students suggested to introduce differences during the group discussion. In order to provide clues for a solution of the separation problem, one duo (variant 3) was assigned to use a fourfold excess of acetic acid. This excess amount reduces the amount of alcohol present after completion to a few percent. Another duo had to use acetic anhydride instead of carboxylic acid. This anhydride produces the same ester and reacts more completely with the alcohol than the corresponding carboxylic acid. For a part this is because the by-product of the reaction of acetic anhydride and alcohol is acetic acid, which can also react with the alcohol to the same ester. These variants, I hoped, would prevent a separation problem from coming into existence.

With hindsight, it is to be doubted whether students are already in a position to understand these rationales, since they do not anticipate any separation problems. And even if they would already understand the equilibrium reaction-type, they could still think that they can get rid of starting reagents by applying separation techniques.

It is expected that students will not anticipate separation problems. When they start with equimolecular amounts of alcohol and carboxylic acid, this will result in an equilibrium mixture consisting of ester, water (the by-product), alcohol, and carboxylic acid. The combinations are chosen in such a way that it will be very difficult to separate the alcohol from the ester with conventional techniques like distillation or extraction. I expected that most students would choose equimolecular amounts, and thus would run into these problems, notwithstanding the fact that, during the group discussion, they were presented with the information on the equilibrium constant.

The table is provided because I expected that this is the information students would want to have anyway. It would take them time to gather these data from literature, time, I thought, could be spent more productively in other ways.

Assignments

During refluxing you execute the following assignments. On the basis of the results you will have to make a plan to obtain a pure ester after refluxing is ended. Thus, find out how you can use the information you obtain from each assignment in this plan.

Assignment 1
In a test tube, mix 1 ml of the carboxylic acid you are working with, with 1 ml of the pure ester you have to make. Observe whether they mix with each other. Add some (tap)water, and write down your observations. Repeat this if you work with two different acids.

Assignment 2
In a test tube, mix 1 ml of the alcohol you are working with, with 1 ml of the corresponding ester. Again, add water. Write down your observations. Repeat this if you work with two different alcohols.

Assignment 3
Do this in the fume board. You will be applying acetic anhydride, which is a hazardous substance. First look up the hazards in a book on laboratory safety.

a) What is the formula of acetic anhydride?

b) Like acetic acid, acetic anhydride can react with alcohol towards an ester. Determine which ester that will be in your case. Write down the reaction equation.

c) Conduct the reaction between alcohol and acetic anhydride by first putting a little alcohol into a test tube. Add a dash of sulfuric acid. Then add a quarter of the contents of a Pasteur pipette of acetic anhydride while keeping the mouth of the test tube away from yourself.

d) Do the same with a mixture of ester and 10-20% alcohol.

Write down your observations and conclusions.

Assignment 4
Measure the refraction index of pure ester. Your teaching assistant will demonstrate how to do this.

Assignment 5
Take an infrared spectrum of the pure ester. Your teaching assistant will assist you.

During the time needed for refluxing, students carried out additional assignments. These were meant to prepare them for the separation and characterization of the end product. They do some test tube experiments to experience the solubility of the alcohol and carboxylic acid they use in water. Some esters can be purified by washing with water. They test the direct reaction of acetic anhydride with alcohol, meant to experience a way to get rid of alcohol if extraction is not an option. They have to measure the refraction index and infrared spectrum of standard esters to get some experience with the apparatus and to experience ways to characterize their own products. After completing these tasks the students have to make a plan for purification and characterization.

Later, I criticized these tasks. The students did not yet have developed the viewpoints from which the tasks make sense. It is not simulation-of-research I was achieving here, it was helping students to purify esters.

Assignment 6
With the help of the information derived from assignments 1 to 5, try to make a plan in which you indicate how to obtain pure esters after the refluxing period, and how you will check whether they are pure. The plans will be discussed with the teaching assistant before you start with the execution. When your teaching assistant has given you permission you can execute your plans. Write down carefully your observations and results.

When you are finished there will be a last group discussion in which you report your findings.

In a third group discussion, purification plans will be discussed. It is anticipated that students do not expect real problems and will propose extraction with water and/or distillation.

The students then execute their plans. They can analyze the results by measuring refraction indices and taking infrared spectra. It is expected that they will find that most products still contain alcohol (which has a very characteristic infrared absorption), except for the two alternative versions (with excess acetic acid and acetic anhydride). It is anticipated that discussion and reflection will lead to an understanding of the relation between choices made in the formation stage and problems in the purification stage.

5.5 A justification of the educational context of Esters

With hindsight, it is possible to interpret the educational design of Esters 1. Esters 1 can be seen as an application of my understanding at that time. In this section I describe the explicit and tacit influences on myself.

Influences from the traditional curriculum (chemical content and topics)

Esters must be seen against the background of the laboratory course M&M1. I was given some liberty to do research in this course. I had the freedom to replace existing organic synthesis experiments by different experiments, if certain organizational requirements were met. For instance, I could not change the time reserved for each experiment or change its position relative to other experiments. Also, I had to make use of the organic compounds and the apparatus available at M&M1. I had to work with the same groups of students, the same TA's, and the same assessment procedures. In short, the alternative had to fit in the empty place. This implied that Esters should be executable within four four-hour lab periods.

The first organic synthesis experiment in M&M1 in 1990 was the one I described in chapter 2: the synthesis of aspirin. I decided to develop an alternative for this experiment. Since the synthesis of aspirin is an esterification, this implicitly drew my attention to the chemistry of esters. Since it would be one of the very first lab experiments, I had to take into account that the first year students would have little or no experience with doing lab work in the field of organic chemistry. That was one of the reasons to start the experiment with a short discussion to make explicit each student's knowledge of and experience with esters, and to start the experimental work with test tube experiments.

Traditionally, one of the most important objectives of lab courses is to provide illustrations of theory and to make students acquainted with laboratory techniques. From this point of view, Esters contains several classical topics. It deals with substance classes such as alcohols, carboxyl derivatives, and esters; with a common reaction (esterification) and an important mechanism (S_N2); and with techniques such as refluxing, extraction, distillation, and infrared spectroscopy. In this respect, the students will not miss anything.

Open, design-oriented experiments

It was clear to me that I did not want to make a cookbook experiment. In a cookbook experiment the prescription determines what should be done. I wanted students to make their own decisions. Although Esters 1 still contains many instructions and prescribed activities, it is open with respect to several elements of synthesis. Students can choose the alcohol-carboxylic acid ratio; they can use a catalyst during refluxing or not; they can choose the purification activities; and they can judge the quality of the result according to standards they have to develop themselves.

The two words 'open' and 'design-oriented' were used to designate such experiments by De Jager and by Goedhart (De Jager, 1985; Goedhart, 1990). De Jager was the first at Utrecht University to study the problems of synthesis education in detail. According to him, 'learning to synthesize' should be the central goal. To him, this meant that students should learn to rationally devise a synthesis procedure. His idea was that students should learn this by designing, instead of just carrying out closed, completely prescribed experiments.

Experiments should thus be open, leaving room for students to make and justify decisions. If the goal is to prepare students for scientific research, the laboratory course cannot restrict itself to recipes in which the mastering of techniques and the illustration of theory are central. De Jager advocated an integration of theory and practice: students should use their lecture course knowledge in the experiments of the laboratory course to make decisions concerning the synthesis procedure.

Synthesis-planning

As I already described above, De Jager developed a theory on how student can learn synthesis which he called 'synthesis-planning theory'. The student should learn to make and justify choices with regard to the whole procedure. De Jager translated this educational issue of synthesis-planning into an experimental laboratory course, in which students had to design parts of procedures. In a first round, he gave a prescription that completely prescribed the formation and the purification, and then had students choose a characterisation technique. In a second round, only the formation was prescribed, and students had to devise the purification procedure too. In the third round, they also had to devise the formation stage, whereas he still provided the names of the reactants to be used and the products to be prepared. In his opinion, students are unable to devise a complete procedure, including starting reagents, since even mature scientists are not able to develop a new procedure from scratch. My design is clearly influenced by this synthesis-planning theory. I prescribed the starting reagents and I gave information on characterization techniques, but I allowed students to devise the purification stage.

De Jager focused on a laboratory course for advanced students, and focused on both organic and inorganic synthesis. Although his ideas had a profound influence on my research, I was uncomfortable with his ideas on the integration of theory and practice. I agreed with his complaint that the laboratory experiments are too often illustration of theory and not application of theory, but the remedy should rather be sought in *preventing* the separation of theory and practice than in integration. De Jager implicitly approves of this separation.

De Jager's conception of 'open' also differs from mine. De Jager made use of blank spaces in prescriptions. For instances, he gave students a complete procedure, but left out the lines in which the specific purification or characterization technique was mentioned. Or, he presented students with a choice between two options. In this way he engaged students in rational reasoning, but he did not achieve a resemblance with chemical research. His strategy resembles a puzzle in which all the pieces are known to be there and known to fit. De Jager seemed to believe that lecture courses ('theory') could provide students with ready-to-hand pieces of knowledge they could use in a laboratory procedure.

I abandoned this approach, because I felt that a theory should be understood before it can be applied. Moreover, De Jager's theory focused on enabling students to design synthesis prescriptions, which is not the same as preparing them for doing research. I had more affinity with Goedhart's ideas on developing theory from experience.

Learning theory from experience

Goedhart investigated the process of learning scientific measuring by first year chemistry students, also at M&M1. He, like De Jager, "rejected detailed and complete instructions and decided to aim at constructing new measuring experiments in which students reason and decide about at least some of the measurement conditions themselves. This might be called a design-oriented laboratory course" (Goedhart, 1990), p. 207). I tried to apply this principle by allowing students to make several decisions themselves. Goedhart also wanted "to develop chemical theory as far as possible in the laboratory instead of solely in lectures and seminars with the aid of the textbook. I expect that this offers opportunities to prevent a gap between theory and practice as observed in existing laboratory courses" (o.c., p. 211). He developed an experiment in which students were to empirically establish a numerical law for boiling point elevation. By doing this, they would come to understand important measuring concepts such as error, dispersion, and the use of graphical representations.

Goedhart's approach in some ways resembles discovery learning. With respect to 'learning to measure' he did not differentiate explicitly between establishing a numerical law and establishing the preconditions for understanding how to establish a numerical law. Although I strongly sympathize with his approach, I was aware of the difficulties of having students construct theoretical insights on the basis of experience. "In the real world of the scientist, theoretical speculation *precedes* experimentation and the search for evidence" (Hodson, 1992b). So, can students design experiments that should also help them to construct theoretical insights? I parted with Goedhart in this respect. In my educational contexts, students should not discover laws or mechanisms or new reactions. Instead, I want to teach to students the issues that enable such discoveries. These issues can be developed from experience. At least, this conviction guided my research: students should discover the prerequisites for doing research in organic synthesis. The criticism that scientific theories never follow from unbiased experimentation therefore does not apply.

Qualitative reasoning instead of a priori calculations

Calculations play an important part in chemistry. But their role is less important than one should think on the basis of chemistry textbooks. Such books often offer the impression that the outcome and the conditions of experiments can be calculated. Elzenga investigated whether students can learn to decide reaction conditions in synthesis and to select, as well as to design, purification techniques on the basis of *quantitative* reasoning, using data and equations from physical chemistry (Elzenga, 1991). He showed that in many instances the applicability of theories taught in lecture courses for establishing reaction conditions such as temperature, concentration, stoichiometry and voltage, is limited. Nevertheless, students often have to perform calculations in the course of synthesis experiments. Elzenga gives an example of an experiment in which students have to calculate the reaction temperature for the reaction of hydrogen chloride gas with solid aluminum to form aluminum chloride. The actual temperature to be used during the reaction, however, is not determined by the temperature at which ΔG is negative, but by the temperature at which the product evaporates from the metal surface. Otherwise the overall reaction rate would be too low. The temperature suggested by the thermodynamic calculation thus is not used in practice. Elzenga concluded that such calculations are mere exercises in calculating. Textbooks help students to perform these calculations, but do not help students in determining the reaction conditions for real reactions. Elzenga thus challenged the possibility of the integration of quantitative textbook chemistry with laboratory experiments. Thermodynamic calculations may make some sense in the field of inorganic chemistry, because of the availability of data on a large temperature range. This makes calculation of the optimum temperature sensible. In organic chemistry, thermodynamic data are not known for many compounds; high reaction temperatures in general are impossible; and the differences in ΔG between a plethora of possibilities are often small enough to allow for many different reaction pathways. This implies that calculation most of the times is not possible or does not predict accurately enough what will happen. Although with the advent of computer-assisted modelling some better tools have become available, even these do not extent towards complete synthesis procedures.

This reflections had direct impact on my research. I focused on students' *qualitative* arguments for decisions, assuming that it is not possible to compute in advance things like reactants, stoichiometry, reaction temperature, reaction time, or amount of product. Nor did I expect students to be able to design quantitative elements of purification activities, such as the fractionating capacity of a distillation column or the number of extractions needed. In Esters 1, for instance, the reactants and the reaction time are prescribed.

Elzenga focused on the use of quantitative *textbook* information. Esters 1, which was designed before I knew Elzenga's work, nevertheless tried to achieve what Elzenga had disproved. I presented to the students the textbook fact that the esterification reactions have an equilibrium constant of about 4, hoping that they would use this information productively in synthesis planning. They did not. However, Elzenga's investigations did not give an answer to the question whether it is possible to apply quantitative data derived from *experience*. He essentially remained within the classical model of separation of theory and practice.

Hermeneutic understanding

In 1990, I did not yet have fully explicated the hermeneutic approach outlined in the previous chapters. However, with hindsight, Esters 1 is in many respects consistent with hermeneutics. When Esters 1 is the application of my 1990 understanding, it seems that I was able to use the issues of learning through experience and of issuing discourse. I also rejected the strategy of conceptual development through transfer of information. Thus, instead of telling the students about esters, esterification, and how to synthesize and purify esters, I had them experience the reactions and the possibilities and problems of purification. By giving students opportunities for expressing their ideas and for explicating their experiences and conclusions I follow the concept of issuing discourse proposed by De Miranda. Group discussions were carefully planned. I also applied the principle of learning through experience to myself: in several instances students were given freedom to do things not anticipated by me, in the hope that students' unconstrained actions would guide me towards a better understanding.

In designing this road I employed other construction criteria as used by the WEI. To create coherence and direction, elements such as questions and assignments should *prepare* students for upcoming assignments and questions. These questions and assignments themselves should have been prepared for by previous ones, and should ultimately build on student previous understanding. To accommodate for students' growing understanding, the educational context could be sequenced into several phases (Van Hiele, 1986). The first group discussion is an *information phase*: the TA is informed about the students' previous knowledge; the students are informed about what they are supposed to do. Ideas and questions are formulated. The next phase, the test tube experiments, is a *guided orientation* to make students acquainted with the chemical context. The second group discussion is an *explication phase*: experiences in the context are explicated. This enables a less constrained *free orientation phase* during synthesis and purification of the esters. Here students can apply their acquired understanding. The purification activity is prepared for by the second set of assignments. However, there is no preparation for this set of tasks itself, which constitutes a potential weakness.

I also planned to look for *productivity*, that is, to determine whether there is a relation between experiences with chemistry, the formulation of these experiences in language, and subsequent successful application. I planned to pay attention to the *meaning* of what students do and say, to disclose the underlying implicit viewpoints. In this respect, I implicitly parted with De Jager. To him, successful synthesis-planning was to be achieved by making rational choices *before* engaging in laboratory activities. He therefore implicitly expected students to already *understand* the issue of synthesis-planning. The students only had difficulty in applying what they knew. I assumed that synthesis-planning is an issue students do not yet understand, and therefore are unable to apply, even if I would give them a detailed explanation. For that reason I prepared a road towards understanding via test tube experiments and various group discussions. The idea of a relation between purification and formation had to emerge from experience before I expected students to be able to apply by themselves.

Understanding needs explication in language. Experiences as such are not sufficient, they should be articulated. In Esters, the students form a group in which different members can explicate, compare and discuss their experiences to reach conclusions and consensus. They are dependent upon each other, for they do not all do the same things, although they have to use the results of others. They therefore have an interest in each others experiences and will not just sit and listen to the reports. They have to be sure that their fellow-students' observations and conclusions make sense because they have to draw inferences from them. The process and the results, both the chemical results and the learning results, are therefore to be granted to the group as a whole, and not to individual students or a collection of individuals.

Educational chemistry

Learning through experiences is possible only if the students actually have experiences. In realistic contexts, it is not always obvious what to pay attention to and what should be regarded as background. It is important that certain phenomena are noticed. De Vos (De Vos & Verdonk, 1985) calls this *educational chemistry*: chemical substances, reactions and phenomena are chosen or created and sequenced for their capacity to induce the kind of experiences that facilitates understanding.

In Esters 1, the reaction is a means to draw attention to synthesis-planning and to the issue of equilibrium. Therefore, those substances are chosen that illuminate these issues as clearly as possible. By letting students compare acetic acid and formic acid, and methanol,

ethanol, and butanol, their attention can be drawn to reaction rate or speed. Mixtures with butanol and/or formic acid react faster than the others, but all are rather slow. This experience could bring students to reflect on influencing the reaction rate, for instance by heating.

When analyzing their crude products, students will find that these still contain alcohol and acid. Acetic acid, methanol, ethanol, and methyl acetate dissolve in water completely, ethyl acetate dissolves partially, and butyl acetate and butanol are almost insoluble in water. Thus, it is possible to wash away acetic acid, but not butanol, from the crude reaction mixture of butyl acetate, whereas it is impossible to purify methyl acetate in this way. Ethyl acetate is an unclear in between. Similar difficulties occur when boiling points are compared for distillation.

The objective is that by comparing the range of experiences with these substances, attention is drawn to the necessity of synthesis planning. The objective is *not* just to make esters, or to get acquainted with refluxing and distillation. Educational chemistry cannot be derived from chemistry qua science, because scientific chemistry *presupposes* understanding. Scientific chemistry is necessary to determine how to make a substance, if that is the goal. The hermeneutic empirical approach is necessary to discover how understanding can be achieved.

The four issues

Of the four issues, only synthesis-planning had an explicit influence on the design. A weakness of my design in this respect became apparent on interpretation. I noticed that I had applied De Jager's synthesis-planning theory uncritically. De Jager stated that a synthesis procedure consists of three stages: formation, purification, and characterization. He was right, but he seemed to have overlooked that this applies to cookbook procedures only. I followed him in this respect. For instance, when the result is known in advance, there is no need to *analyze* crude products, the results of distillations, etc. It is possible to wait until the product is completely purified and then do a final characterization to prove the identity. In the experiments of De Jager, students were supposed to fill in blank spaces in otherwise complete cookbook procedures, by rational a priori reasoning. I wanted students to make choices not only on the basis of a priori reasoning but also on the basis of experiences. I realized that students therefore had to know the composition of crude mixtures, but I did not realize that this in fact means the introduction of a fourth activity: analysis. I did not give students the appropriate tools for analysis, I only gave tools suitable for the characterization of an end product, such as infrared spectroscopy and refraction index measurement. If I had been able to *apply* my knowledge of what happens in chemical research (after all, I graduated as an organic chemist) when you do not yet know a successful procedure, I would have realized that some form of chromatography would have been far more appropriate. I apparently needed to go through the cycle of Esters 1 before I understood this, and, hence, was able to apply the issue of simulation-of-research in the design of educational contexts.

On interpretation, I also discovered that several assignments did not accomplish what I had expected them to do. Students executed the tasks, but they did not make a productive use of the experiences. I realized that this had something to do with the structure of the educational context, in which students are given instructions without first evoking a question on the relevance. This understanding gradually developed into the issue of simulation-of-research. Esters 1 was designed without using the issue of simulation-of-research. In several respects it was an uneasy mixture of openness and prescriptions.

In the next sections, I will continue with a more detailed analysis of the empirical findings of Esters 1.

5.6 A description of actions and events

Before analyzing in detail what happened regarding the four issues I give an overview of actions, discussions, and events. This description is not meant to be complete in any sense. I intend to draw a sketch of the context in which actions and discussions to took place, to give a background to the details I present below.
The experiment started with a group of eight students, a TA, and me, in a room adjoining the laboratory. The prelab group discussion was held, in which students told what they knew about esters. They were told that a goal of this experiment would be to make esters. Students then conducted the set of test tube experiments. They made mixtures of the acids and alcohols and noticed that it is difficult to detect what is going on. It took some time before a faint, probably ester-like smell developed in some of the test tubes. These experiences were discussed in the second group discussion, along with other things that were brought up by the students. As a result, consensus was reached that a good way to prepare esters is to heat them in a reflux apparatus using sulfuric acid as a catalyst. Each duo of students then went to the laboratory to synthesize two esters. One pair of students covertly received some extra information: they were told to use a fourfold excess of acetic acid. Another duo had to use acetic anhydride instead of acetic acid. All students set up the reflux apparatus without much problems. During the refluxing, they performed the second set of assignments. They did some test tube tests on the solubility of esters and learned to use the infrared spectrophotometer and the refraction index apparatus, using pure esters and alcohols from stock. The TA's gave a short explanation on infrared spectroscopy. For instance, the attention was drawn to a specific absorption around 3500 cm^{-1} which is present in alcohols but not in esters. Some students already managed to analyze their crude product. On the basis of these findings the students reflected on how to obtain the pure esters. The TA set a time limit on the refluxing and assembled the students for the third group discussion. Students proposed and discussed purification methods; mainly extraction and distillation. The TA commented on their plans and in the last laboratory round students executed their plans. Some extracted, some distilled, and all analyzed their products with infrared spectroscopy. The results of this were discussed in the last group discussion. It is against this background that I will present and analyze specific actions and discussions concerning the four issues.

5.7 Reaction-type

The development of the issue of reaction-type was not a point of view to me in the design of Esters 1. I assumed that the students would know that the reaction taking place when alcohols and carboxylic acid react to form esters is an equilibrium reaction. I expected that students would understand the issue of equilibrium, that is, that they would realize that the starting reagents will still be present after the reaction had reached its endpoint. However, I did not expect that the students would understand synthesis-planning. That is, I expected that they would try to get rid of the remaining reagents with purification techniques instead of using an excess amount of acid. Esters 1 was designed to develop this understanding of synthesis-planning by choosing combinations of substances that would make purification with distillation or extraction virtually impossible. This experience, I hoped, would, upon interpretation, draw attention to the issue of preventing the problem by taking appropriate measures in the formation stage.

My assumption thus was that students would not use their knowledge of the esterification reaction being an equilibrium reaction, for synthesis-planning. From this viewpoint it seemed appropriate to give them the information on equilibrium in advance. During the second group discussion, that is, after the first test tube experiences but before deciding on the amounts of starting reagents to be used, the TA explicitly wrote the equilibrium formulation on the blackboard:

$$K = \frac{[\text{ester}][\text{water}]}{[\text{acid}][\text{alcohol}]}$$

Before that happened, some things had occurred that made me wonder whether students really understood equilibrium. During the prelab group discussion, the question how to make esters was breached:

TA If you .. ethyl acetate .. is an ester .... if you want to make that .. how would you do that?
a3 Ethanoic acid and ethanol? And then .. yes ..
a8 And then just wait and see.
a2 Yes.
(laughter)
TA Yes, okay.

This short discussion is just what was to be expected. The answer corresponds with the question. From this context of question and answer it cannot be inferred whether students know that putting together an alcohol and a carboxylic acid leads to an equilibrium mixture and also to the by-product water. The student did not mention a complete reaction equation and the TA did not ask for one. I initially supposed that those issues were left unspoken because they are obvious and trivial. However, during the test tube experiments, I noticed they were not.

During these reactions, I noticed that many students first rinsed their test tubes with water before using them. They did not dry them! In the context of esterification, such a 'cleaning' is counterproductive, because the remaining water may diminish the quantity of ester being formed. A student who knows and understands the equilibrium reaction-type would not do this.

I noticed that some students executed the test tube experiments as follows. They measured off as exactly as possible the quantities mentioned in the manual (1 ml); they put the liquids together; they put the test tube in a rack and finally wrote in their lab notebook equations like:

$$\text{ethanol} + \text{acetic acid} \rightarrow \text{ethyl acetate}$$

I then asked questions:

R Tell me, what have you been doing?
a5 I have made methyl acetate.
R The methyl acetate is in this test tube?
a5 Yes.
R Is it all methyl acetate?
a5 Yes.
R Nothing else?
a5 No. Well .. I am not completely sure if I measured off the stuff all right. But it should all be ester now.

This took me by surprise. However, not all students did agree:

a2 Well ... I don't know. It looks like nothing happened.
R Why is that?
a2 Well .. you don't see anything. It looks just like water .. just like it was. It is just colorless liquids. I don't know. I think nothing happened.
a3 It does not smell like esters. It stinks.
a4 Well ... perhaps we used too much of that acetic acid. Not the right amount. That's why it still is so .. so .. pungent. But I think it is ester. Did you smell it?
a5 No.
a4 Here .. [smells the test tube of a5] .. aaahh .. just as bad as mine.

Only one test tube, the one that contained formic acid and butanol, seemed to develop a sweet smell. Somewhat later, the students added some sulfuric acid to the test tubes. This led to the generally experienced phenomenon of sweet smells. They compared this smell with glue or nail polish remover. In many cases, students reported that a stinging acidic odor was still present.

These test tube reactions were meant to draw students' attention to the fact that esterification reactions are quite slow. They seemed successful in this respect. However, they also drew my attention to the fact that many students seemed to disregard the equilibrium notion. I conjectured that students may be inclined to think that the reaction would proceed to completion; some even seemed to think that it would happen instantaneously. I use the verb 'to think', because this is the usual way to say these things. But in fact students do not consciously have any concept of reaction-type in mind at all. By using the verb 'to think' I try to indicate that I can make sense of students' acts and statements by assuming that their understanding, and hence their application, is implicitly guided by such viewpoints.

My hypothesis now is that students use the prototypical reaction-type conception $A + B \rightarrow C$. That is, they base their actions and interpretations on the implicit assumption that, in principle, the reaction comes to completion and produces only one product, the ester. On reflection, it seems to me that this conception may be an effect of students previous experiences with the role of water and with synthesis. The majority of secondary school chemistry experiments involve water as a solvent. This gives water a role on the background: it is always present but does not receive any specific attention. The students may ignore water not only because they have no attention for by-products, but also because they automatically locate water on the background.

With respect to synthesis, the students do not have a history of trial and error with synthesis. It seems natural to focus on the product. In education, the experiments and

syntheses that are demonstrated are always successful; and success in synthesis is identical with making the product. Why start a synthesis when you know that it will not work? The students are not acquainted with a context in which putting together reactants does not automatically lead to the desired result. Of course, students know about equilibrium, but equilibrium is an issue in acid-base calculations, not in synthesis.
Nevertheless, the experiences make clear that there is no instantaneous transformation into 100% ester. The students seem to explain this from the viewpoints of speed and stoichiometry. At least, that is consistent with what they do and say. On speed:

b3 Reactions don't proceed ah .. complete.
TA No?
b3 So if you do bigger amounts you have .. ah .. lots of product .. yes .. that doesn't react.
TA Yes.
b7 Then you have to use a catalyst.
b3 Yes, we did that.
TA That was the acid, you know, that is what we tried.
b7 Yes.
b6 Maybe temperature?
TA That's a great remark!
b4 Yes, good idea.

As a result, the students used a reflux apparatus and they used sulfuric acid as a catalyst. On stoichiometry:

a4 I think it is very important, the right ratio.
(...)
a1 If the ratio is wrong, something will be left.
a2 So there's too much left and then you can't smell it because that other substance dominates.

So, if the stoichiometry is all right, and if the reaction is granted enough time or is speeded up, the end product will be there in 100% yield. As a result, all students (except those students who had to do an alternative version) took pains to start refluxing with the exact molecular stoichiometry. This interpretation is consistent if the students expect to end up with 100% pure ester after refluxing. I think they do, but is difficult to determine this issue. The difficulty is caused by the design of the educational context. I will pick up this issue again in the next section.
With regard to the reaction-type issue, I noticed that students kept focusing on the ester as the one and only product. The by-product water was ignored completely. For instance, water is not mentioned as one of the substances present in the crude synthesis mixture that need to be removed from it. And, many students 'cleaned' their glassware with water. However, a coincidence drew students' attention to this issue. The synthesis of butyl acetate, which starts with a homogeneous mixture of butanol and acetic acid, leads to a two phase system. This phenomenon was experienced as a surprise in need of interpretation:

b4 Yes ah .. that is some sort of mixture, over there ...
b3 Yeah .. that upper layer, it contains that ah ..
b4 ..ester.
b3 ..ester with a little butanol in it.
R Why is there still butanol in it?

b4 Hasn't yet reacted I think.
b3 No .. ah .. yeah.
b4 We had butanol as starting .. there was another such layer .. well .. that has to be something .. it can't be that 2 millilitre of sulfuric acid that we added.
R No.
b3 So there likely is...
b4 Oh, oh .. water! Can that be, can it?
b6 Water?
R Is it only ester that is formed?
b3 Yes .. there also is water!
b4 Woh!

It seems to come as a revelation. A piece of information the students had known all the time suddenly became part of an experience and was understood. They move away from the prototypical reaction-type $A + B \rightarrow C$ because the mechanical separation into layers does no longer allow them to implicitly regard the product as having just one chemical identity.

Although they established water as a by-product, they still have problems with understanding why butanol is still present. The students have washed the reaction product with water and analyzed the upper layer, first by measuring the refraction index, then by taking an infrared spectrum. They discuss this:

b6 But why still butanol?
b3 Why not?
b6 Because everything reacts with acetic acid.
b3 Yeah ... maybe there is too little acetic acid?
TA Well .. it .. ah .. there always is a reaction constant, isn't there? So there always remains something of the .. substances. From which you started.
b3 So all that stuff with measuring that index was for nothing. So it means that it isn't pure, that ester.

B6's statements indicate a viewpoint on reaction from which reagents are completely transformed into products. B3 starts to explicate an idea, but is unfortunately interrupted by the TA, who forces attention to equilibrium. The students' were probably on their way towards attention for equilibrium anyway. Before this discussion, b3's understanding and activities seemed to have been guided by the presupposition that the reaction product must be pure. This presupposition now is disclosed, making understanding possible.

Such dialogues made clear to me that this issue of by-product formation as well as the issue of equilibrium deserve explicit attention in the redesign of the educational context. In designing Esters 1, I had not anticipated which problems this lack of understanding could cause. For instance, some students, making ethyl acetate, purified their product by way of distillation. They expected that this would work well. However, the infrared analysis revealed the presence of a hydroxy-group. This led students to believe that the product still contained alcohol. Although this may be true–and it certainly was the conclusion I hoped they would draw–the absorption could also have been caused by water. In general, the samples were dried with magnesium sulphate before using the infrared apparatus (to protect the NaCl windows of the infrared cells). But I observed that this drying was often done superficially or even omitted when students had distilled instead of washed. They simply did not expect water to be present. On interpretation, I had to admit that the design was not working adequately.

5.8 Synthesis-planning

I used De Jager's synthesis-planning theory explicitly when designing Esters 1. The explicit intention was to make students understand the usefulness of synthesis-planning by confronting them with a purification problem that could have been prevented by making appropriate choices regarding the formation.
However, as I already described in the previous chapter, I was not able to circumvent several inconsistencies. Esters 1 takes for granted the cookbook-like subdivision of procedures into separate stages. I planned a formation stage (refluxing), a purification stage (extraction, or distillation, or whatever the students would propose), and a characterization stage (infrared and refraction index). Analysis during formation and analysis during purification was not planned.

I will first pick up again the issue whether students do or do not think that during refluxing the reaction comes to completion. This issue is difficult to decide upon because the educational context was not explicitly designed to find an answer to this question. I explicitly programmed several activities meant to prepare students for the purification stage. The student manual states: "Make a plan in which you indicate how to obtain pure esters after the refluxing period, and how you will check whether they are pure". In the group discussion following this stage, the TA's explicitly ask students *how* they want to purify their product. Not, *whether* they want to purify at all:

TA Now tell me .. what was your idea of obtaining the pure substance?

In such a context, I now suppose, students automatically take it for granted that they have to conduct purification activities. In Esters 1 the question was never raised explicitly whether the student really think that their crude product contains anything but ester and are in need of purification. But I have some reasons to think they implicitly do. Neither the TA nor the students attempts to specify or quantify the impurities. They seem to employ the principle that nothing is ever perfect, thus, when you start with alcohol and acetic acid, the final result can in principle contain these substances. Consequently, purification is normal. They have never seen a synthesis that was not followed by purification. Thus, the students respond:

a6 Well .. we assume that in the reaction product .. ummm .. everything contains that we threw into it .. plus what reacted ... should have been formed .. the ester.

This assumption could have been a starting point for a discussion: "Why do you assume that?"; "How much will have been left of the starting reagents?"; "Which final purity do you want to obtain?". However, these questions were not raised. The students thus engage into activities without clearly defined expectations or goals. In this way, purification is little more than a ritual. The only exception is sulfuric acid. The students realize that this additional substance will still be present after the reaction is completed. With respect to the alcohol and the carboxylic acid, they seek a technique which will remove these substances in principle, present or not. This ritual purification, they trust, will then assure complete purity.

So, after an extraction or distillation, the students characterized their products, and expected to find absolute purity. This behavior is consistent with their school chemistry experiences: experiments are always successful; activities like distillation are meant as an illustration of the activity. They see no contradiction. They do not notice the inconsistency of executing token distillations and extractions in this context. Therefore, it is necessary that the students learn synthesis-planning not just as a way to relate stages in a procedure, but also to learn the very idea of controlling a procedure from the viewpoints of yield and purity.

I, however, made an analogous mistake when choosing identification techniques like infrared and refraction index for analysis of crude mixtures. These techniques are always applied at that stage in (cookbook!) experiments. Since I apparently did not understand this issue, I did not program an analysis of the mass balance of the crude reaction mixture during or directly after refluxing. The sequence I planned was refluxing-purification-characterization. Consequently, the students were not able to reflect on the necessity or quality of their purification efforts, because they obtained no data on previous stages. Moreover, they received conflicting information on the purity of their products. Measuring refraction indices and infrared spectra is excellent for pure substances, but the results are difficult to interpret in case of impurities. Some students reported a refraction index of the purified product very close to the value of the pure ester, whereas the infrared spectrum showed the presence of substances with a hydroxy-group and the product itself still smelled after acetic acid.

I had expected that measuring an infrared spectrum would be revealing because the presence or absence of alcohol would be revealed by the intense hydroxy absorption around 3500 cm^{-1}. Almost all purified products contained a huge absorption at this place. However, I had not expected the attitude of students towards water. Although in the group discussions the group reached consensus on the interpretation that the products contained alcohol, this conclusion is not completely warranted. On interpretation, I became aware that the techniques I had chosen were inappropriate. The students should have started analyzing their products much earlier, using more informative techniques.

Although the educational context was not successful in all respects, I could confirm the hypothesis that students were not able to apply an understanding of synthesis-planning with respect to relating purification to formation. All students chose stoichiometric ratios. When they became aware of the impurities, they tried to solve the problem by trying new separation techniques or by repeating the same technique. That is, they tried to solve the problem by looking forward, instead of by reflecting on the previous stage. Of course, in many cases it is appropriate to use additional separation techniques. But this educational context was explicitly designed to urge the necessity of reflection. The students simply were unable to reach a result that satisfied their own (implicit) objectives.

One student had washed the crude product of the ethyl acetate synthesis with water. He expected to get rid of sulfuric acid, acetic acid, and ethanol in one time. Since ethyl acetate is somewhat soluble too, he lost quite a bit of the crude product. On infrared analysis, he experienced a huge hydroxy absorption, which was interpreted as resulting from ethanol (because the sample had been dried with magnesium sulphate). He repeated the washing procedure, again lost half of his product, but did not achieve a better result. He refused to wash another time, afraid of losing all product. He now turned to me:

a4 What do I do now? It does not work.
R What?
a4 I have washed this two times with water, and it still contains alcohol. And I have lost almost everything.
R Well .. quite a problem. And distillation [pointing at some students who are distilling]?
a4 I have been thinking about that. But they [refers to another duo] have tried that already, and they had the same .. the same thing .. spectrum .. as me. Also alcohol. I don't know. And I have looked at the boiling points but they are almost the same.
R Now what do you want?
a4 Get rid of the alcohol! If only there was a substance with which I could react it away.
R Which kind of substance?
a4 Well .. I don't know. What reacts with alcohol ... sodium or something?
R What do you ... react with sodium ..?

I was so surprised that I did not know what to say. Why could he think of sodium and not of acetic acid? It seems that it is very difficult to reflect on the context of formation when you are busy in the context of purification. In the words of another student:

b6 To look back on what you have been doing ... you just don't think about that.

At this moment, I nevertheless thought that my educational context was working quite well. Attention was drawn to a very difficult separation problem that apparently could not be solved with conventional methods. I was waiting for the duo that was working with excess amount of acetic acid. I expected that they would be able to make esters that did not contain alcohol. I knew that this was possible from my own preparations for this experiment. I had been able to make and purify products without hydroxy absorption. Unfortunately, I made three mistakes.

The first mistake was that I over-estimated the students manipulative skills. They were completely new to such techniques as extraction, distillation, and drying. This had an influence on yield and purity. The second mistake was a trivial problem of relative quantities. The student manual stated "Conduct the reactions with 30 ml of acetic acid". The students doing the alternative version were told to use a ratio of 1:4. This implied using just 12 ml butanol, which in turn resulted in a much lower absolute quantity of ester (theoretically about 17 ml) than I thoughtlessly had anticipated. The students conducted the same purification activities (washing with water, distillation) as the other students and were unacquainted with these techniques. They made some mistakes themselves too, and so most of their product was lost. In both groups, only very little product was salvaged for analysis. On the smell of it I was sure that it was the ester, and I hoped it would lead to convincing experiences. But then my third mistake intervened. The purified product may have been free of alcohol, but it was not free of water, since there was not enough to dry the distillate with magnesium sulphate. So in both cases the infrared spectrum revealed a clear hydroxy absorption. There was no honest way in which I could make them interpret this spectrum differently, so consensus was reached that this sample contained alcohol too. The next fragment comes from the final group discussion:

b3 Butyl acetate.
TA Butyl? Which ratio's?

b3 One time 1 to 1, and the other 4 to 1 .. of acetic acid 4.
TA So 4 .. I'll write it down on the blackboard. .... And?
b3 In the ratio 1 to 1 we had a lot of product .. and the other was little. Mm .. from the infrared spectrum it appeared that both were very .. or .. that they contained alcohol.
(...)
b2 Well .. you hope that the acetic acid will ah .. completely reacts the alcohol away .. and he doesn't do it.

The student indicated that he understood the rationale of adding excess acetic acid, but this was not reinforced by experience. However, I was convinced that it could be done, if I redesigned the educational context appropriately.

In the other group, a break-through almost occurred. During the group discussion the students working on making butyl acetate and butyl formiate made proposals regarding purification. The following discussion took place:

TA But .. assume that it does .. ah .. alcohol in the ester .. ah contains?
a6 Yes ah ..
TA That may happen. And .. what do you think to do about that?
(silence)
a7 Adding extra water that ah ..? Extra acid .. shake well .. ahh ...
R Extra acid, did you say?
a7 Yes that ah .. reacts towards ester with water.
R With alcohol?
a7 Yes.
TA That would be .. to repeat a piece of synthesis, in this case.
a7 Yes.
TA Yes, that is .. when you are separating the end product .. it is a trick of course .. but it is not completely .. the intention. There is, in fact, there is another way. I have just looked at the Table to see if it is feasible .. and it is very well feasible .. namely .. just look at the boiling points of methanol, ethanol, butyl acetate and butyl formiate.
(silence)
TA Yes? What is drawing attention?
a6 They are far apart.
(silence)
TA So?
a6 Distillation in that case.
a7 Yes.
TA Right.

The remark of a7 ("extra acid") came out of the blue, and I jumped on it immediately. However, I was completely overruled by the TA, who apparently had drawn his own plans. The chance was missed. I did not notice on the spot that the TA actually made a mistake. He should have compared with the boiling point of butanol (instead of ethanol and methanol), which is very close to the boiling points of both the esters.

It is very easy to blame the TA. However, that would be unfair. He was just trying to make the best of it in an educational context he had never experienced himself. He followed my suggestions as if they were strict guidelines, to make sure things happened according to plan. This experiences made me reflect on the role of the teacher. I realized that my teaching objectives were not sufficiently clear. Also, the educational context was too much directed towards making esters, instead of towards learning synthesis-planning.

Synthesis-planning is also related to the technical and theoretical limits of the various techniques available. For instance, if it were possible to separate ethanol and ethyl acetate in a normal distillation apparatus, it would not be necessary to use an excess amount of acetic acid during formation. I noticed that students seemed to over-estimate the possibilities of the equipment. In Esters 1, students seldom spoke about their quantitative expectations regarding yield and purity (because they were not asked to say anything on these matters). Indirectly, I got the impression that they expected 100% yield and purity to be normal. They did not reckon with loss of yield due to practical problems or theoretical limits.

b7 We just want to wash it with water a few times, so you are sure that the esters are pure.

Their high expectations can be explained from their inexperience with synthesis techniques. They often did not know or understand the theoretical foundations of a technique. Distillation is regarded as a technique for separating liquids that have a different boiling point. How this separation takes place is not understood. Consequently, they regard distillation as a black box, unconstrained by technical or theoretical limits. For instance, they seem to think that the vaporizing process starts at the boiling point of the independent component, and that each liquid vaporizes independently of the others. Therefore, they do not understand the place of the thermometer in the distillation apparatus, and they also seem to expect that any difference in boiling point, however small, will suffice for distillation. In the next fragment, a student reports on her efforts to purify methyl acetate:

a5 It didn't work perfectly .. there was some methanol in it .. so it wasn't pure ester .. and yes, how did that happen, that is the next question. Yes .. I think it is because the thermometer was not hanging in the liquid .. that had to be kept at 57 degrees .. but ah .. about 5 centimetres above .. in the gasses that were hanging there .. and .. ah .. the liquid for sure was a little bit warmer .. and .. ah .. methanol has a .. ah .. a boiling point of 65 degrees .. and the ester of 57 degrees .. so there's only 8 degrees in between .. so I think ah .. because that temperature of the liquid was higher .. yes .. some alcohol is evaporated too .. and that is why there is .. alcohol in the product.
TA Yes .. that about that thermometer ..
a2 Where exactly was the thermometer?
a5 Yeah it was about 5 centimetre above the liquid that ah..
TA ..yes and with respect to the condenser .. where was it?
a5 Yes right in front of it.
TA Yes ah .. what ah .. do you intend to measure with that .. thermometer?
a5 Yes ah .. I thought .. you got ah .. down in the flask you got ah .. a fluid with all kinds of stuff in it .. among them that ester, you know .. and that ester when it still is a liquid .. is liquid .. because it has to be brought at 57 degrees, and then it goes evaporating .. then he goes .. then the vapor rises and then, yes, he will reach the thermometer .. but ah .. I thought .. that it could have been a little bit warmer .. but yes .. well .. maybe not .. I don't know.

Such dialogues occurred with surprising frequency. For instance, another student wanted to separate butanol and acetic acid (both with a boiling point of around 117-118°C) from butyl acetate (b.p. 126°C):

b4 Distilling ... see .. we have to go to the boiling point .. to heat it about 119°C .. do we have to do that with a flame?

TA No, you can just use an electric heating mantle.
b4 I see .. yes .. but you cannot adjust them very well.
(...)
b4 How can you get that heating mantle at 118? No .. I don't mean .. you can get him at 180 and higher .. but how do we get him at exactly 118 degrees?

In general, students regarded controlling the temperature of the boiling liquid as crucial for achieving a good distillation result. They had no attention for other limitations. They assumed that all substances behave as if they are independent from one another. In this context, however, the formation of azeotropes severely hampers the possibility of purification through distillation. For instance, a mixture of ethanol, ethyl acetate and water has an azeotropic boiling point of 70°C, with a azeotrope composition of 82.6% ethyl acetate, 8.4% ethanol, and 8.0% water. This result is incomprehensible to students from the point of view of the independent-substance conception. More details on this issue and on the problems of learning distillation in general can be found in a separate study on distillation (Van Keulen, Goedhart, Mulder, & Verdonk, 1995).

With respect to extraction, students also seemed to think that this technique has two options only: either it separates completely, or it does not work at all. This conception was put into question by their actual experiences, which were far removed from this prototypical expectation. This was one of the rare instances in which the specific washing assignments mentioned in the student manual seemed to achieve anything at all. Most students just executed these tasks and did not combine the experiences with their purification efforts. One pair of students, however, noticed that a few drops of water could dissolve completely in a mixture of ethanol and ethyl acetate. A little bit more resulted in a two-layer system. Adding yet more water eventually led to a one-layer system again. They were intrigued, but did not reflect on their experiences, because the separation problem had not yet become an issue. Later, they thought about purifying their crude ethyl acetate product and remembered their experiences. They repeated the tests, to make sure that adding a specific amount of water led to a system in which they thought they could separate the ester from the acetic acid:

a4 Umm .. from assignment 1 and 2 it was clear that ah .. ethanol and acetic acid dissolve well in water and ah .. the ester doesn't. So I ah .. wanted to mix it with water so as to dissolve the ethanol and the acetic acid, and ah .. the ethyl acetate .. that has a smaller mass than water .. will float on top.

Since they knew that ethanol and acetic acid mix well with water, they concluded from seeing a two-layer system that ethyl acetate did not dissolve. They implicitly assumed that, in this system, all the ethanol is in the water layer, whereas all the ester is in the other layer. This assumption was contradicted by the actual experiences with washing the crude mixture, as I described earlier in this section.

I had provided another explicit clue for solving the purification problem. This clue was hidden in the assignment in which students had to add acetic anhydride to a test tube containing both ester and alcohol. When doing this, they could observe vigorous reaction phenomena. In the student manual, I explicitly stated that a reaction occurs in which the same esters are formed. I hoped that students would use this reaction when they would have discovered that extraction and distillation would not lead to alcohol-free esters. To reinforce this, one duo was assigned to carry out a synthesis starting right away with acetic anhydride. However, nothing came of my plans. Although all students conducted the test tube reaction and wrote down a reaction equation, nobody ever gave the slightest hint of combining this with the rest of the experiment. The task had not been prepared by previous discussions or experiences, and it apparently did not prepare for an application, too. The students using acetic anhydride in their synthesis did not achieve results, either. One of the students decided to quit university, leaving an incomplete synthesis behind. In the other group, the crude product disappeared in litres of water used for extraction and was never recovered.

On interpreting, I realized that my idea of evoking this solution overstretched students' anticipations by far. They did not yet have an expectation of purification problems, and they were not yet able to reflect on the formation stage. They did not yet have developed an applicable reaction-type concept nor an applicable understanding of synthesis-planning. As a consequence, they had no interest in an analysis of the mass balance of the mixture, nor did they see the activities in which they were engaged from the viewpoint of controlling a process to satisfy norms regarding yield and purity. Let alone that they were able to combine these two viewpoints. Moreover, using a reaction to prevent a purification problem is a shift of context. To students, chemical reactions occur in the formation stage; in the purification stage, physical processes are employed, but chemical reactions do not take place anymore.

5.9 Structure-activity-relations

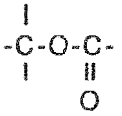
As I already mentioned, the issue of structure-activity-relations did not exist to me as an *educational* issue. Establishing relations between molecular structure and activity, I thought, is what happens in real chemical research. Students should be prepared for doing research, but not by some sort of discovery learning in which they, like researchers, have to discover real chemistry. So I figured that, when you would want to make esters, even if you knew the molecular structure, it would be too difficult for students to suggest starting reagents. I decided to connect with students' previous knowledge on esters: they already know that esters are made from alcohols and carboxylic acids. I did not plan to let the students reflect on this fact. So the question why alcohols react with carboxylic acids played no role in the design of Esters 1. It was during the interpretation of Esters 1 that I realized that I should differentiate between the ability to *answer* such questions–which is an issue in chemical research–and the ability to *ask* such questions, which, I came to think, is something to be learned through education and through reflection on education.

One of the prerequisites for being able to ask questions is that you realize that there *is a relation* between structure and activity. From the way students talked about substances, I got the impression that they more or less equated substance and structure. In the prelab group discussion, the TA started a discussion on students' previous knowledge on esters and esterification:

TA I hope everyone in any case knows what an ester is. I mean .. what the characteristic of an ester group is. Who?
a4 It is ah .. carboxylic acid and ah .. alcohol.
TA Yes .. that was already the second question .. that is how you make an ester .. but what is the characteristic ester group?
a3 C .. O .. C .. and then on that one C a double bond with O.

TA Could you perhaps draw it on the blackboard? I think it is superfluous but you never can write down such things often enough.

a3 [writes on the blackboard:]



$$-\overset{|}{\underset{|}{C}}-O-\underset{\underset{O}{\|}}{C}-$$

TA I assume that everybody knew this. Well .. how do you make an ester, you said it already, you just connect ah .. an acid .. an organic acid with an ah .. alcohol.

To both the TA and the students, this dialogue seemed to have a matter-of-fact quality. The line of thought seemed to run from the word 'esters' towards the question 'what is characteristic of esters' to the answer 'a certain combination of atoms in a structure'. However, instead of this last sentence, it seems that I can also fill in 'a certain combination of symbols on paper'. There was no apparent reference to substance properties of ester, such as esters being colorless liquids with a sweet smell. Nobody seemed to feel the need to relate the molecular formula with macroscopic properties. It seems as if the paper formula is more real than the substance itself. It is interesting to note that a4 initially refers to what can be called the history of an ester: an ester is the substance that comes into existence when an alcohol and a carboxylic acid are combined. The TA explicitly separates this property of esters from what he regards to be the real essence of esters: the characteristic string of atoms. The students apparently seem to accept this move.

It seems that what results are two sets of unrelated facts. On the one hand, the fact that alcohols and carboxylic acid react towards esters, on the other hand, the fact that these compounds can be written in a symbolic formula language. The specific string of symbols occurring in esters is a characteristic *label* by which one can recognize esters. The students do not understand the *functional* relation between the two. The label could have been *any* string of symbols without this changing the course of the experiment. The TA did not raise the issue, perhaps could not raise the issue because the educational context was not yet prepared for drawing attention to the issue of structure-activity-relations.

This did not satisfy me. I combined this reflection with my findings on the use of acetic anhydride. The students were able to find the molecular formula of acetic anhydride; they could write down a reaction equation of the reaction with alcohol; but they could not apply this in the context of synthesis and purification. To them, the reaction between alcohol and acetic anhydride was just another fact. It did not automatically make them interpret their experiences in the light of the functional differences between the acid and the anhydride. The structure-activity-relation I implicitly tried to employ was that, in the case of a nucleophilic attack by alcohol, the anhydride contains a better leaving group than the acid, and thus may react more vigorously and completely. The reverse reaction is hampered, too, since water is a better nucleophile than acetic acid, the by-product in the anhydride reaction.

I tried to make students use this reaction in the context of purification. With hindsight, it is understandable that students were quite unable to follow my line of thought. If anything, I should have tried to use the difference to draw attention to the structure-activity-relation as such, in the context of formation.

Since no student made any comment whatsoever on acetic anhydride, this piece of educational chemistry apparently was not understood. The context and the viewpoints necessary to see the use of acetic anhydride as a solution to a problem had not yet been developed. I realized that it would be better to elaborate on what I had been trying to achieve with sulfuric acid. In the test tube experiments, students first make mixtures of alcohols and acetic and formic acid. They notice that the mixtures containing formic acid are the first to develop a noticeable sweet odor. Adding sulfuric acid speeds everything up. During the second group discussion, my attention was drawn to this order:

R What is the function of sulfuric acid?
a1 It goes faster.
a2 It goes to its equilibrium faster. [the TA has just mentioned the equilibrium equation of the esterification reaction, including mentioning $K = 4$]
R Yes. In which way?
a3 I think .. those H-plusses .. go immediately ...
R Sulfuric acid generates the H-plus?
a3 Yes .. and maybe it takes in an H-plus also .. so he .. ah .. comes off quicker.
R Acetic acid ... formic acid isn't that too ah .. can also generate an H-plus?
a1 Ummm .. it is weaker.
R Yes. Considerably weaker.
(silence)
R Which one is weaker, acetic acid or formic acid?
a4 Acetic acid.
R Acetic acid.
a1 That is a difficult question .. I think .. the longer the carbon chain is ...
a2 I think formic acid, it is stronger.

It is clear that it is me who is drawing attention to this issue, but a1's remark on the influence of the length of the carbon chain started my reflection on structure-activity-relations. At least, students understand one such relation: they understand that carboxylic acids contain a COOH-group that is responsible for the acidic properties. This draws attention to the qualitative relation between the molecular formula and substance properties. But quantitative differences in acidic properties have to be explained too, and in the context of the molecular formula there seems to be only one possible cause: the length of the carbon chain.

Perhaps students are able to develop an understanding of the 'esterific' properties of these substances if I could make them elaborate on such observations. I tried to redesign the educational context in such a way that I could pay attention to this issue.

5.10 Simulation-of-research

Simulation-of-research can be a successful approach when it is taken as a point of view by both the designer, the teacher and the student. Neither was the case in Esters 1. The TA's had no experience with supervizing open experiments; the students had no experience with doing them. Both had problems with their roles. And I did not provide enough help. For instance, from the point of view of the students, it is consistent to ask "What do we have to do now?" when they just have completed a set of 'assignments'. The same holds for the TA's. On the one hand, I wrote in the teaching manual that I wanted them to "listen to the students, and be careful with telling 'how it works'". On the other hand, in the same manual, I gave very explicit directions: "The expected conclusion is that all esters can be separated by washing with water, except methyl acetate. The test tube reactions with anhydride can demonstrate whether any alcohol is left in the product. In the case of methyl acetate it will be necessary to distil". I cannot blame the TA's that they did not always know when to be observant and listening, and when to give explicit directions. This resulted in such dialogues as:

TA Okay .. we are going to make arrangements on ah .. what we all are going to do. Umm .. the majority indeed will wash .. ah .. with water. And ah .. in the end .. I know .. only one distillation was necessary .. let me have a look on what it was exactly .. tuddum .. let me look .... only methyl acetate was not possible, it says here ... let's have a look whether we had that here too .. ah .. who was doing methyl acetate?
b1 Umm .. weren't we? Yes.
TA You?
b1 Yes, we were stuck with that methanol.
TA And that was ...
b4 Hey .. so *we* did that wrong, with that distilling.
TA It appears that ah .. notwithstanding what you were thinking ah .. if ah .. if b3 and b4 just add water .. then, according to the manual, it will work just fine.

This was the kind of discourse I wanted to prevent, but I apparently failed to achieve this. As I explained, I could not improve much concerning the starting situation of the TA's. So I had to settle with this kind of discourse occurring now and again, since the transmission-of-knowledge strategy as such would not help the TA's to understand their role any better.

However, with hindsight, I realized that my own contribution to the TA's and the students inability to achieve more productive discourse was important, too. My intention with Esters 1 was to develop an 'open, design-oriented' experiment. That is, an experiment in which students could make their own decisions so that they could understand the rationale of synthesis, especially with respect to synthesis-planning.
My experiences with the way students conducted the second set of test tube tasks made me realize that I had been inconsistent. My experiences with the infrared apparatus made me realize that I had implicitly modelled my experiment after synthesis *prescriptions*, instead of after research. My tasks prepared students for reaching the correct chemical solutions, whereas they should prepare students for understanding the underlying issues in organic synthesis. Instead of giving tasks and assignments, I should design a context in which experiences and problems draw students' attention.
Many student-activities and statements in Esters 1 make sense from the points of view of their previous experiences with chemistry education. For instance, the special position of water, the independent-substance conception, the equation of formulae on paper with chemical substances, and the expectation of total chemical success with reactions and purifications are learning results of previous instruction. This implies that building on previous knowledge can not always be effective. My open, design-oriented approach implicitly builds on previous knowledge because it does not always explicitly reveal this knowledge as problematic in the (new) context. When students execute assignments, they suppose they will get credit for a correct execution of the assignment itself. My intention was to pose a problem, or to induce a cognitive conflict, but my approach was not very successful. A problem-posing approach that is more consistent with my intentions is *simulation-of-research*; this is also in accordance with the fundamental objective of preparing students for doing research. The open, design-oriented approach implicitly

builds on a conception of education characterized by instructions and prescriptions and on a conception of chemistry characterized by facts acquired through previous instruction. *Simulation-of-research is an approach that builds on a conception of education characterized by issuing discourse on the basis of explicated experiences, and on a conception of chemistry as a research activity based on questions and hypotheses.*
When making esters is turned into a research problem, several questions can draw attention. The focus can be on the practical procedure itself, but also on theoretical explanations and mechanisms. Yield and purity can be used as indicators for success with regard to developing a practical procedure, but they can also be used to answer theoretical questions. Both points of view influence synthesis-planning, since both frameworks can suggest different activities and pose different norms for yield and purity. For instance, to investigate the equilibrium character of esterification, it can be revealing to compare the effects of using an excess carboxylic acid with using an excess alcohol. From the point of view of developing a practical procedure, the use of an excess alcohol should be avoided.

If I had explicated this issue of simulation-of-research to myself at that time, I could have formulated conditions for redesigning the educational context. However, I was not yet thinking in terms of simulation-of-research. Instead, I tried to enlarge the open character to give students more freedom and responsibility to ask and answer questions. To achieve this, I introduced in Esters 2 assignments and techniques that were more functional, but still in a task-like manner. This is described in the next chapter.

6 Understanding

6.1 Changes in the educational context

On the basis of my interpretation of Esters 1, I understood that several changes in the educational context were necessary. A first change was that I left out everything concerning acetic anhydride. I furthermore changed the test tube experiment as follows:

> 1. Prepare in (marked) test tubes the following mixtures. Use about 1 or 2 centimetres of the substances.
> a) methanol plus acetic acid
> b) ethanol plus acetic acid
> c) 1-butanol plus acetic acid
> d) methanol plus formic acid
> e) ethanol plus formic acid
> f) 1-butanol plus formic acid
>
> 2. Prepare 8 test tubes; 4 with 1 cm ethanol and 1 cm acetic acid; and 4 with butanol and acetic acid.
> Add 5 drops of sulfuric acid to the first test tube; 5 drops of a concentrated sodium hydroxide solution to the second; a few grains of nickel powder to the third; and a few iodine crystals to the fourth. Do the same with the test tubes filled with butanol and acetic acid.
> Stir the tubes and place them in the rack.
> Write down your observations. Compare with the observations from 1.

I anticipated that using more than one 'catalytic' substance could make student reflect on the question why it is sulfuric acid that has such a dramatic influence, whereas the other substances do not influence the process. Explicit attention to sulfuric acid could draw attention to the role of the proton and hence to mechanistic features. Such discussions, I hoped, would provide opportunities for studying the development of structure-activity-relations.
The refluxing stage remained essentially the same. I still anticipated the students to propose to rise the temperature during the reaction. I expected that nobody would object when the TA would allot combinations of alcohols and acetic acid. So, the first duo would use methanol and ethanol; the second ethanol and butanol; the third methanol and butanol; and the last ethanol and butanol; whereas all would use acetic acid. The last duo would be informed to use a fourfold excess of acetic acid. Instead of telling the students to use 30 ml of carboxylic acid, I now prescribed 50 ml of alcohol. So students using an excess acid would not end up with very little ester. I also wrote in the student manual:

> When the mixture is refluxing, immediately take a sample of about 1 ml with a Pasteur pipette. Take more samples during refluxing. These samples will be analyzed in assignment 4.

'Assignment 4' was one of four assignments meant to be done during refluxing. In Esters 2 I still thought I should include assignments that would suggest clues for reaching good chemical results. The first two of these were again on making test tube mixtures and observe what happens when water is added. This task prepares for extraction. The third assignment was again on measuring the refraction index. The fourth one replaced the assignment on infrared spectroscopy. Instead, I let the TA demonstrate a gas chromatograph (GC), using pure esters and some purpose-made mixtures of esters, alcohols, and acids. I took explicit care to avoid suggesting that the students' samples and crude products eventually would also contain alcohol and acid. On the basis of these tasks, the students were again supposed to make a plan for obtaining pure esters from their reaction mixtures. This plan would be discussed in the third group discussion.

I also gave some different guidelines to the TA. I told them to focus explicitly on students' theoretical ideas concerning the reaction between alcohol and carboxylic acid, when this issue would be raised. Such discussions, I hoped, would help me gain a deeper understanding of students' understanding of structure-activity-relations (although I did not yet use that term). I did the same with respect to equilibrium: when students would use this word, the TA was supposed to probe this notion. In current terminology, I hoped to confirm my hypothesis that students on the one hand *know* about equilibrium, but on the other hand are unable to *apply* such knowledge productively.
I told the TA's that the students were free to deviate from the directions given in the student and teacher manual when this seemed appropriate to them. I told them that I anticipated that the students would agree with ideas such as heating the reaction mixture and analyzing samples; they just do not know the appropriate chemical techniques. For that reason I gave the instructions on refluxing and gas chromatography directly in the student manual.

To a very large extent, things happened as I had anticipated. The test tube experiments draw students' attention to theoretical, mechanistic questions concerning the esterification reaction. These issues were discussed and explicated at length in the second group discussion. Even the question whether or not the reactions form equilibrium mixtures was discussed. Nevertheless, all students again opted for stoichiometric ratios when designing their syntheses. The analysis of samples with the gas chromatograph worked well. There were some initial problems with interpreting the chromatograms, because the highly polar substances water, sulfuric acid and carboxylic acid could not be detected by the device used. The esters and alcohols under consideration, on the other hand, could be detected within minutes. Most students concluded that the ratio of ester to alcohol in their crude reaction mixtures was in the order of 2 to 1 (in units corresponding with peak surface). The students using excess acetic acid, however, obtained a far better ratio. In the third group discussion, these different results led to lively discussions, inducing several students to also use excess acetic acid. Others thought they could purify with distillation or extraction. Eventually, only those who used excess acid obtained almost complete purity, whereas the others did not.

6.2 Reaction-type

In Esters 1, I was unsure whether students knew (that is, had learned in secondary school) that the esterification reactions under consideration are equilibrium reactions in which water as a by-product was formed. In Esters 2, students mentioned these facts already in the first group discussion:

TA Okay. Next, the concept esterification. What does that mean?
d1 That is a reaction.

d4 That is a ah .. hydrolysis .. water is released.
TA Yes, how? Ummm ... hydrolysis between what?
d4 Ah .. an acid and an alcohol, for example. And then water is released and an ester.

And:

TA Does this always work?
(...)
c3 Equilibrium of course.
TA What is it?
c3 Equilibrium.
TA Which equilibrium?
c3 Well .. if you put it together, then ah .. yeah ..if it is to the left, the equilibrium ...
TA Yes?
c3 Then you need another temperature .. but ..
c5 You have to heat it, I thought.
TA Why do you have to heat it?
c5 Well .. otherwise the reaction does not .. ah .. take place. Maybe it has something to do with the ah .. enthalpy .. that T must be higher to take the reaction towards the right.
(silence)

These facts could be remembered by students from secondary school textbooks. Most of these books contain an equation:

$$\text{ethanol} + \text{acetic acid} \xrightleftharpoons{\text{heat; } H^+} \text{ethyl acetate} + \text{water}$$

Students apparently remember fragments of this piece of information.

d4 Shouldn't we add that catalyst? H-plus, I think.
TA H-plus? Is that necessary?
(silence)
TA Why should that be necessary? I mean .. you said: just put it together?
d2 Yes, and look whether it happens .. if it happens it is okay, but if it doesn't you have to figure out something different.

It seems that students knew relevant facts, but were not able to produce a convincing rationale. I concluded that the upcoming test tube experiments were in accordance with students previous knowledge and ideas.

In the second group discussion, the students discussed equilibrium on several occasions. For instance, one student mentioned that the contents of one of his test tubes did not smell like esters at all. He added water to the test tube to clean it, threw into a waste container, and then smelled the ester:

c2 ...and then, when I rinsed it .. it suddenly got that ester smell.
(...)
TA Yeah .. but what do you think will be the effect of adding water?
c4 That it actually shifts the equilibrium to the *left*.

This last remark is a very accurate conclusion. However, not all students explicated their experiences in terms of equilibrium. There was consensus that the test tube reactions did not lead to the best results: although some tubes developed a smell characteristic of esters, they all still had a distinct acid smell. To explain this, some students used the equilibrium concept. Others held that the reaction was not yet completed:

c4 Yeah that reaction, hasn't it such ah .. such an equilibrium from two reactions .. the forward and the backward. And it may be that it just .. by the ester-reaction .. that you simply do not supply enough warmth to get over that activation energy, so the reaction simply does not proceed at all.
(...)
c6 Yes listen, if it is equilibrium than it is no use to wait for a long time because the amount of ester being formed stays the same because that reaction .. ah..
c5 Yes but it can increase .. maybe it is not yet in its equilibrium because it goes so slow.
(...)
c2 Yes .. it might be an equilibrium with a threshold or something .. somewhere it must get over a threshold value. A certain energy.
c5 Activation energy.
c2 Activation energy, yes. When it cannot get over that, because you do not heat it ...
(...)
c1 You have an equilibrium extreme left, haven't you .. the bigger part is left.
c5 That is also possible.
(...)
c3 You cannot shift something when you do not have an equilibrium.
(several students speak together)
TA Wait a moment ...
c5 An equilibrium that you can form more quickly than when you have room temperature, okay .. then he will go faster. Or the equilibrium simply shifts.
c3 But is unlikely that it is equilibrium because the pure ester exists too. Otherwise it would be formed back immediately.
c4 Of course! If you have equilibrium and you remove that water then you only have just that reaction to the right .. going to that ester .. and if you go on removing the water then there is a moment that you only have ester.

In a lively, heated discussion, in which the TA hardly participated, c4 formulated a chemically excellent procedure for making esters. However, there appeared to be no intention to actually remove water during the reaction. This proposal seemed to be a construction meant to reconcile the idea that the reaction is an equilibrium with the fact that pure esters also exist. The statement nevertheless made me wonder whether a proposal to add extra acetic acid could also have been made. Probably not, since removing water is an act of purification anyway, whereas adding acetic acid seems more like introducing an impurity. In any case, she didn't convince the others:

c2 But when you put esters into a jar .. and there is vapor .. water gets in and immediately you do not have pure esters anymore?
c4 Yes, that is true.
c6 And you can store the esters, so ...
c4 Yeah, yeah .. that is generally the case.

On interpreting such discussions I realized that students probably had very limited experience with slow reactions. In secondary school, chemistry classes last only one or two hours, and teachers cannot afford to waste time demonstrating slowly progressing reactions. Instead, almost always reaction mixtures are demonstrated that react instantaneously. Heating is employed for those mixtures that otherwise would not react spontaneously at all.

Students do have some secondary school knowledge of equilibrium, but this is in general restricted to mixtures already in a state of equilibrium, to enable calculations. Van Driel (Van Driel, 1990) has shown that in most secondary schoolbooks treatments non-equilibrium situations are omitted. In thermodynamics terms, the (non-equilibrium) equation $\Delta G = \Delta G^0 - RT\ln Q$ is taught incompletely because only equilibrium situations in which $\Delta G_{eq} = 0$ and $Q = K_{eq}$ are dealt with.

In this context, students noticed that mixtures of alcohol and carboxylic acid apparently are stable. So they concluded that this situation either is "an equilibrium extreme to the left", or it is a situation in which the reactants need to be heated for reaction to take place. One pair of students did actually heat one of the test tubes that did not smell sweet with a boiling water bath:

c6 We heated it .. for five minutes at a hundred degrees .. and the acid smell was gone and you could detect an ester smell.

This observation provided enough ammunition to those students who did not explain their experiences with an equilibrium concept, to convince the others that heating would enable them to change the reaction mixture entirely into ester. This was the outcome of the second group discussion: heat the mixtures and add a catalyst. All students chose stoichiometric ratios; no student attempted or suggested to remove water from the reaction mixture. So the discussions on equilibrium had no consequences for synthesis-planning in this respect.

However, in defend of the students, I should also say that it seems to be far more difficult to develop and apply an understanding of the equilibrium concept than I had expected. In the first place, it still is possible to interpret the experienced phenomena in different terms. In the third group discussion, one pair of students reported on their GC analysis results after using a fourfold excess of acetic acid in their reactions. Most students eventually had an ester peak with a peak surface area of about 60-70% of the total surface area; the other 30-40% belonged to the alcohol. With excess acetic acid, the ester to alcohol ratio was considerably higher.

d3 Well .. you take the same amount of acid and you got the same ah ..
d8 No, we had 4 times as much acid as ah .. as alcohol. And it was .. with butanol it was 99.2%. So we already have more than 99%.
TA Yes, that GC percentage is not exactly correct, but in any case it is quite high. What does that imply for the reaction, when you see that ah .. with you .. not so much reacted .. and .. that with adding extra acid .. indeed .. ah .. large amount of ester is formed. What does that suggest?
d3 Equilibrium.
TA What do you think? Is that right? Is that what you expect if it is equilibrium?
(silence)
d6 Yes.
(...)
TA Does everybody agree?
d1 I don't know.
TA You still have doubts?
d1 It doesn't need to be equilibrium, does it?
(...)
TA Why wouldn't it be an equilibrium reaction, d1?

d1 Ah .. when you just have more acetic acid in it .. and at a certain moment almost all ah .. alcohol is gone .. and then there also is almost no acetic acid .. if you would do it 1 to 1. So equal amounts.

TA And why wouldn't there be any acetic acid left?

d1 Because all the acetic acid reacts with ah .. with the alcohol.

TA You have 4 times as much.

d1 No, if you wouldn't do that. In that case .. the chance that they would meet each other is much smaller, so it will react ever more less, and if there still is a lot of acetic acid, than the alcohol will easier .. meet an .. acetic acid .. molecule .. so they can react more easily. So you can have more yield.

TA Ummm ..

d6 It isn't that crowded inside.

This statistical argument appeared difficult to refute. D1 adds other arguments:

d1 It also is not sure that it is equilibrium because it is not sure that if I would throw in more ester .. will that result in more acid? That is not proved.

(...)

d1 Well .. maybe if I would wait a couple of days .. maybe I would also get something close to 90 per cent.

(...)

d6 But you said .. if the reaction is running out .. and you .. you said that if more of one substance is added that he will go to the other side. But if it is running out then everything must be to the other side?

d1 No .. that is why it is running out: less and less gets formed.

d6 Yes but ...

d3 It must be running out, it can't be equilibrium.

d6 But then .. it doesn't matter if you add one of the substances?

d1 Why not?

d6 Because ..

d1 Running out doesn't mean that everything reacts? It means that less and less reacts. And in the end there is so little left..

d6 But that is equilibrium.

d8 Yes.

d1 Yes, it is equilibrium.. at a certain moment there is this amount of substance and this amount of substance .. but it isn't slowly shifting.

d7 That is equilibrium, isn't it?

d6 Yes!

d1 No, equilibrium is when it also goes backwards.

According to d1, it still is not convincingly proved that this is not just a slow reaction. However, his last statements suggested an experiment. In the next laboratory round, the first thing d1 did was to set up an experiment in which he heated a mixture of ester, water, and sulfuric acid. Within minutes, the characteristic stinging odor of acetic acid developed. This convinced him. In my observation notebook I wrote that he "engaged in research-like activities". I thought this was one of the most successful moments of Esters 2. I wrote: "If I could get students to formulate their own questions, then it may not be necessary to give them assignments". This reflection developed into the concept of simulation-of-research. In my opinion, this student was doing research. It may be true that chemists already knew the answers, still, the combination of argumentation with experimentation lies at the heart of chemical research. D1 had a rationale and checked it empirically.

A second problem hindering students in interpreting their experiences in terms of equilibrium has to do with their previous experiences with equilibrium equations. These originate chiefly from the context of acid-base chemistry. In this context they have learned to omit the concentration of water in formulae. A typical equation has the form $HA + H_2O \rightleftarrows A^- + H_3O^+$.

This leads to the formula: $K_a = \dfrac{[A^-][H_3O^+]}{[HA]}$.

Many students tried to use such a formula in this context too:

c1 May I say something? Ah .. the formation of an ester is an equilibrium, isn't it? Yeah .. I just ask .. it is equilibrium. Well .. the entropy becomes smaller .. yes .. first you have 2 particles .. that becomes 1 particle.
c4 No, why should it? You also have water.
c1 No .. water is .. is liquid .. you know that.
c4 Yes, you say: water is liquid .. but the other three substances too ..
c1 Yeah..
c6 Yes, no, but water does not participate in the ah ..
c1 Water does not participate.

In the other group, a student actually wrote down the consequent formula:

d7 We are dealing with this reaction [writes on the blackboard]:

$$C_2H_5OH + CH_3COOH \longrightarrow H_2O + C_2H_5OCOCH_3$$

$$K = \frac{[\text{ethyl acetate}]}{[C_2H_5OH][CH_3COOH]}$$

d1 What has happened to water?
d7 What?
d1 Water.
d7 That never appears in an equilibrium constant.
(silence)

These discussions took place at the end of the experiment. Although the students who thought that water in this context should be included in the formula managed to convince the others, a tacit understanding to exclude water could have hindered students in an earlier stage to interpret their experiences in terms of equilibrium:

d3 Actually, it cannot be equilibrium because when you have ester .. when you try to get it out .. it will fall apart again.
TA What?
d3 Ester itself would set up an equilibrium again.
d4 If he has water.
d3 If he ..?
d4 If there is water.
d3 Yeaah .... okay.

Students sometimes apparently possessed the knowledge to refute or correct certain conclusions, but this only happened when tacit presuppositions were explicated, like here. But that was not always the case.

A third reason for students not to apply an understanding of equilibrium to synthesis-planning has to do with lack of experience with the application of formulae in chemical contexts. Students have a lot of experience with solving numerical exercises in which equilibrium constants or concentrations have to be calculated. So it seems conceivable that they would apply this knowledge. However, I noticed that it was out of their reach:

TA And why did you take 6 times as much?
d1 Because they used 4, and .. well, I have a higher yield than they had the first time.
(..)
TA Yes. And 5 times? What would work best?
d2 Yeah .. you should just try that.
d1 Just try it, yeah.
TA How would you try it?
d1 Well ah ..
d2 2 times as much, 3 times, 4 times, 5 times.
(...)
TA Are there other ways?
d1 Calculation.
TA How would you calculate it?
d1 I have no idea.

Although students have experience with textbook equilibrium calculations, these exercises in general consist of two or three quantities given and a third or fourth that has to be calculated. In the context of this experiment such experience does not suffice. In chemistry education, chemical reactions often merely provide a background for solving equations that are purely mathematical in character. Here, things are far more complicated. An essential difference between paper exercises and experimenting is that in the first context the data are unambiguously given, whereas in experimenting the data are constituted by an experimental technique. To use the data, it is necessary to understand the way data are constituted. When a technique is regarded as black box, this poses problems. This issue can be illustrated by elaborating on the process of interpreting the chromatography data in order to apply them in synthesis.

First, students have to realize that, in principle, it is possible to estimate an equilibrium constant from the data they have at hand. If they assume that the GC surface areas ratios correspond approximately with molecular ratios (an assumption that has no physical ground but merely is a convenient approximation), then they can transform the ester to alcohol surface ratio of about 65:35 to a 2:1 molecular ratio. This assumption only holds if the sample is at equilibrium, and if the equilibrium constant is not too much affected by temperature. They have to realize that the correct equilibrium formula also contains water and acetic acid. They have to figure out that these will have the same ratios. This leads to an estimation of K of about 4, which accidentally is surprisingly close to actual figures (Sarlo & Svoronos, 1990). This in turn could be used to calculate the excess amount of acid necessary to reduce the quantity of alcohol, but only if the students would impose a purity norm upon themselves. This whole operation involves considerably more than straightforward calculation. A numerical textbook calculation leads to a correct answer but has no consequences for experimentation. In this context, however, the result of the calculation is to have a functional relation with experimentation. Here, the context of simulation-of-research could provide the reasons for experimentation and/or calculation, because it engages students in the quest for maximum purity as an expression of the quality of the method. The quality of the chemical result can be influenced in a controlled manner. But to exert this control it is necessary that the students understand synthesis in terms of a combination of yield and purity. To achieve, say, 98% purity, it is necessary that the yield of ester also is 98% with respect to alcohol, since it is almost impossible to get rid of the alcohol otherwise. Calculation can help to obtain the desired purity and thus can prevent experimentation by trial and error.

I discussed this calculation with students during lab sessions, trying to coax them to proceed a little bit along this route, but without success. I got blank faces in response to my questions and suggestions. As Elzenga (Elzenga, 1991) already had concluded, students' textbook knowledge does not enable them to quantify reaction parameters. The best they could do thus was to follow their intuitions for choosing an excess amount and to set up trial and error experiments, as is illustrated in the previous transcript.

So students eventually applied and understood a qualitative notion of the equilibrium reaction-type. What is more, the questions related to this issue inspired them to engage in the formulation and testing of hypotheses. In this way, they were able to establish, in the context of synthesis, what it means that an esterification reaction is equilibrium, and how to relate this to synthesis-planning. However, a quantitative understanding was not achieved. The students' viewpoint of 'purity' seemed to give rise to an absolute, unquantified meaning. A quantitative understanding would enable students to transform the qualitative reaction-type $A+B \rightleftarrows C+D$ into a quantified one of the form $xA+1B \rightarrow (x-0.98)A+0.02B+0.98C+0.98D$. Such a relation would expresses a quantitative norm for the quality of the result: 98% purity. In this way, calculation becomes part of the educational context; learning to calculate becomes a contextual development.

So far so good. If it takes such an effort to develop an applicable qualitative understanding of equilibrium, what does this imply for other reaction-types? For instance, students never seemed to make an issue of the possibility of side-reactions or subsequent reactions. The results of Esters 2 with respect to the issue of reaction-type suggest three consequences to be explored. First, are students able to apply the equilibrium reaction-type in a new educational context? Second, will they relate their reaction-type understanding to qualitative synthesis-planning? Third, is it necessary and possible to expand their understanding of reaction-type towards other types? And fourth, is it possible to integrate such a contextual development in a context of simulation-of-research, in order to prepare students for application of these issues in their future careers?

6.3 Synthesis-planning

Initially, I reserved the issues of synthesis-planning for understanding the relations between the stages in synthesis. I gradually understood that this interpretation was too narrow. Decisions regarding relations between stages as well as decisions concerning a single stage are both related to synthesis as a whole. For instance, the decision to use an excess amount during the formation is related to the possibilities of purification. But the exact excess ratio is also related to a desired result. In the case of esterification, a fourfold excess makes sense only if a purity of 98% is desired, otherwise it would be wasting acetic acid.

I realized that students had to make several decisions concerning just one stage, or concerning the end result. For example, heating the reaction mixture or adding a catalyst in themselves do not lead to higher purity or better yield in this specific case; it is only in relation to a desired duration of the experiment that such notions are important. Students (and chemists) do not want to waist time. The search for conditions that speed up the reaction rate is part of chemical research, too. It seemed appropriate to take into account such one-stage parameters.

I did not attempt to focus on all possible relations between desired result and synthesis-planning. I excluded (in this study) economic and social factors like cost and waste, which also influence synthesis planning. This is because chemical theory in general falls short in deciding such issues. For instance, chemistry alone does not tell which compounds are toxic to humans, or expensive. I restrict myself to study the teaching and learning of *chemical* reasoning.

In this respect, the attention drawn to heating reaction mixtures belongs to synthesis-planning. After the test tube experiments, students had no doubt that heating the reaction mixture is beneficiary. However, they implicitly seemed to have different rationales. Speeding up a slow reaction is one reason; another is to enable a reaction that is thermodynamically impossible. This is already dealt with in the previous section. Students, however, were mainly interested in the issue of speed; they wanted to know whether the reactions would proceed without heating or not:

c6 Yeah we could try that experiment another time and heat until you see something.
c3 You also could heat one tube tonight and another just .. leave it as it is .. and one we could put it in the fridge or something.

Although this kind of synthesis-planning seems a little bit trivial, it can also lead to attention to the other issues. Just as the success of using an excess amount of acetic acid begs for an explanation, so does the success of heating.

In Esters 2, the educational context was better equipped for developing an understanding of synthesis-planning. The replacement of infrared spectroscopy by gas chromatography helped significantly. Through their experiences with the test tube experiments, the students' attention had been drawn to the problem of reliable analysis. They wholly agreed that looking at colorless liquids or sniffing at stinging odors was far from ideal. The proposal to take and analyze samples using a device unknown to them therefore met no objections, although the choice of GC was not a result of the students' discourse but was an assignment from the text.

The students were already acquainted with the fact that chromatography is a technique for separation, but they were ignorant regarding the underlying principles. The TA very briefly explained these principles, with an emphasis on differences in vapor pressure and on differences in interaction with the column material of components in the mixture. The

settings of the devices used were already attuned to the samples to be analyzed. The students only needed to inject their samples. Chromatograms were electronically processed, integrated and printed; these prints included retention times and peak surface areas, both absolute and as a percentage of the whole. A set of chromatograms of the pure alcohols and esters was made available, so students could compare the retention times of these with the retention times of peaks in their samples. In this way, they could identify the substances present and they also obtained an estimation of the relative amounts.
Treating gas chromatography as a black box had the disadvantage that students initially had to rely on the TA for interpreting their chromatograms. Due to low column temperature, high interaction with the stationary phase, and low flammability, acetic acid, sulfuric acid, and water never appeared in the chromatograms. This at first confused the students. They also tended to equate relative peak surface areas with absolute molecular quantities. Hence, the TA needed to help them interpret their chromatograms. Nevertheless, the chromatographic analysis of the samples, although little understood, served its main purpose, that is, to give students sufficient information on the composition of their samples. More information proved not necessary, and therefore I did not turn to another technique. After the third group discussion, during the purification stage, students were able apply the technique independently.

In the third group discussion, the results of the GC analyses were discussed and interpreted. All students had started synthesis with stoichiometric amounts, except the students that were assigned to use excess acetic acid. All students saw an increased ester-alcohol ratio when comparing their first and last samples. They compared their results with other students in the cases in which the same starting reagents were used:

TA Yes .. wait a moment .. I want that peak .. the ethanol peak .. no the ester peak in the case of ethanol .. to compare yours with theirs.
c2 Mine is ..
c8 We did ethanol.
c3 We too.
TA Okay, I want that too.
c2 We got 99 point 03%
TA Ester?
c2 Ester, yes.
c8 99 point ...?
c2 99 point 03
(surprised whistles)
c5 That it almost the pure stuff.
(...)
TA Can I get the others? I am ..
c8 Ethanol?
TA Yes, ethyl acetate.
c2 Yes, ethyl acetate, 99%.
TA He got a main peak of 99%.
c3 72.
TA 72.
c8 64.
TA 64%. And that is .. after how long? Is that more or less the same? More or less the same time .. refluxing? Do you know?
c2 I did 5 measurements .. so I have .. 2 .. about one hour and a half.
c8 I did 7 measurements.

c3 Yeah, we too. Two hours.
c8 So we got approximately the same period. Still, a difference of 8%.
c3 But you had only one hour and a half, yes? But you have more result, that is clear.
c2 That is right, because I used excess acid.
c16 What was the ester peak in the beginning?
TA When you took a sample for the first time. What was the percentage of that one?
c2 Nothing. Zero.

Almost similar discussions occurred in the other group. The experiences with excess acetic acid led the students to reflect on the particular reaction-type and to conclusions regarding purification. Just as in Esters 1, the students first looked ahead: they suggested to distil and/or to extract with water:

TA Well .. it is intended that you will ah .. purify the mixture you have made. (..) Does anybody have an idea?
d3 You could distil it. It is different boiling points.
(...)
d8 You also could add a lot of water. In that case ah .. the acetic acid stays in the water .. and the ester with the alcohol will float on top of the water.
d6 Yes.
d7 You can remove that .. pour it off or something .. or with a small pipette .. and then in any case you have got rid of the acetic acid.
TA And then?
d7 And then distil, likely, because then there is a very big difference between them.

The students again seemed to expect that butanol and butyl acetate could be separated completely by way of distillation. However, they realized that it is not possible to treat ethyl acetate and methyl acetate in this way, because they had found through the assignments that these dissolve in water. Moreover, the differences in boiling point between ester and alcohol are even smaller in these cases.
At this moment they started to make use of the results of the excess synthesis:

c3 We could also work with excess acid of course.
c8 We could ah .. could try to ah ..
TA Wait a moment ..
c3 Ethyl acetate..
TA Yeah.
c3 You could add excess acid. That ah .. then .. well .. the ethanol would be ah .. used .. what is left now .. because .. look ..ah .. acetic acid has a boiling point of 117 I think ..
c8 Yes.
c3 And the other 78, isn't it?
c8 Ummm .. below hundred I think.
TA In any case considerably lower.
c3 So it could be possible, I think, with distillation.
TA Yes.
c8 Because then you have an ah .. a mixture of 2 compounds and one has 117 boiling point and one has 77. And then you can distil. So with an excess acid you remove the ethanol you still have .. you remove that.
TA Yes.
c8 Into ester.
TA Okay. And suggestions for methanol .. or .. yes .. methanol?
c3 Same. The same.

As a result, some students added extra acetic acid and let the mixtures reflux again before further purification. Others thought they could get rid of the other substances through direct extraction or distillation. In the end, only those who treated their crude mixtures with excess acetic acid achieved a satisfying purity.

c4 We had .. we started from the fact that it wouldn't have reacted completely .. something like one mole of alcohol would be present. So instead of that ratio of 1 to 1 we calculated in the beginning we now just made sure that .. from the starting situation .. when we had thrown in everything .. that we would have 3 times as much. So .. but something had reacted already, so we had more than 4 times as much.
TA Excess.
c4 Excess added. And we had .. we let it reflux for more than an hour ... and we had 100% methyl acetate.
TA But are you sure that you have 100% pure ester in your jar?
c4 No, surely not.
TA Well, what is in it, then?
c4 It is .. well .. it was not detected by the gas chromatograph .. but .. that can't be completely 100% accurate.
TA What do you think is in it?
c4 In any case .. acetic acid .. it contains water that isn't detected.
c3 Sulfuric acid too.
c4 And sulfuric acid.
c1 Yes and contaminations and what ..

It was also found that the ester-alcohol ratio was hardly influenced by washing and/or distillation.

TA Ah .. butyl acetate? Who have been doing that one?
d3 We.
d6 We too, yes.
d4 We had 100%.
d7 Yeah, we too had 100%.
TA And you?
d5 98 point 8.
d3 I have .. well .. I probably did that reaction wrong .. I had .. with OH-minus I had it ah .. well okay .. distilling didn't work.
TA Of butyl acetate?
d3 Yes.
TA Didn't work, distillation?
d3 Didn't work with me .. I got 70%.
TA 70%.
d3 Little .. yes .. something 70 or 68 .. and then I thought: well, I'll try it with NaOH.
TA Yes.
d3 Ah .. 4 mole per litre .. I washed it .. I got 2 separations .. I thought maybe that proton reacts of ah .. the one who is attached to the O with ah .. butanol .. reacts maybe with OH-minus .. and then you get .. you get .. it dissolves .. this butanol ion dissolves in water .. will dissolve .. and then ah .. you can pour it off. But I don't know how much.

It is interesting to note that the last student, who was the only one in his group not to use extra acetic acid, tried to apply one of the very few structure-activity-relations that is applicable on the basis of the secondary school curriculum. However, butanol is not a very good Brønsted acid since it is a very bad proton donor, and the success of the extraction operation was limited. I will return to this issue in the next section.

The results convinced the students that using excess acetic acid was the best thing to do. Most students also achieved excellent chemical results. They probably understand this aspect of synthesis-planning by now. This is a hypothesis that can be tested in a subsequent educational experiment.

I was less satisfied by the way I still gave several prescriptions. Gas chromatography was introduced by the TA and by the student manual without much problems. The same held for the assignments on extraction. It seemed to me that it was not really necessary to prescribe these activities. Several of the transcripts I reproduced reveal that the students apparently had sufficient attention to the issue of purity. Their goal in this experiment was to make esters. Students apparently presume that a little bit of a very pure ester is closer to this goal than a large amount of an impure mixture. From the students' point of view, purity dominates yield. My hypothesis thus is that students are already able to explicate the wish to analyze samples and to try to purify by washing with water. Perhaps it sufficient to ask a few questions on analysis and purification during group discussions for these issues to receive attention, and to leave out explicit assignments. During the group discussions, the TA then can inform the students of the technical details of chromatography and extraction.

6.4 Structure-activity-relations

In the redesigned educational context I explicitly wanted to focus on structure-activity-relations to determine the starting point of the students and the possibilities for elaboration. Initially, students appeared to use molecular formulae as labels. Formulae have characteristic groups that determine the *name* of the substance, not its properties. However, students already have a certain experience that a formula can also represent chemical properties. This stems from their experiences with Brønsted acid-base substances. The fact that acidic or basic properties can be represented by proton donating or accepting structures is well-known from secondary school. Experiences that elaborate on this seemed to promote enhanced understanding of structure-activity-relations. In Esters 2, I will demonstrate this with a very lively, ongoing discussion on the function of sulfuric acid in the esterification reaction.

The students were discussing their experiences with the test tube experiments. They agreed that the tube containing butanol and formic acid developed the most ester-like smell, more so than butanol and acetic acid. But butanol and acetic acid aided with a few drops of sulfuric acid reacted even better. The opinions on using nickel or iodine were mixed; some students thought it might work, but they did not argumentatively defend their view. The comparison led to attention to questions underlying the effect of sulfuric acid:

c5 That sulfuric acid, I see something of an explanation for that, but not for the rest. You know .. with that nickel and iodine .. I have no idea how that would work as a catalyst.
c2 Iodine may be. Because it dissolves.
(silence)
R So how do you see that with sulfuric acid?
c5 Well .. that sulfuric acid takes away the H_2O that gets formed .. and it becomes HSO_4^- and H^+ .. that meets that H_2O and .. because that H_2O is taken away it goes again .. becomes .. the reaction proceeds to the right again .. proceeds.

R Which H_2O?
c3 The faster, the better..
c6 ..the reaction product of the formation of ester.
c5 Yes. And that is taken away by H_2O and therefore more ester gets formed.
(silence)
R So what does the rest of you think of this?
c3 Umm ..well .. could be, yeah .. that it works as a catalyst, that's what you say?
c5 Ah .. yes. Well .. ah .. not as ah .. as .. it does not stay H_2SO_4 but it splits up into HSO_4^- and H_3O^+ and then ..
c6 Gets used in the reaction.
c5 Yes.
c4 It splits for sure. It's a strong acid so it is split up.
c5 No, there was not yet any H_2 .. what is it .. there was not H_2O yet. It was a pure substance. At least, that's what we assumed, it was pure, wasn't it? So there was no H_2O and that H_2O arrived only when the ester got formed. And then it could split up. And then that H_2O disappeared and then more ester could be formed.
(silence)

The students experienced that sulfuric acid speeds up the reaction. They know sulfuric acid as a strong (Brønsted) acid: a proton donor. So it is understandable that they try to explain the effect of sulfuric acid through its proton. According to the Brønsted theory, proton donors react with proton acceptors. From all substances present, there is only one substance of which students know that it is a proton acceptor: water. So c5 tries to explain the effect with what organic chemists would call a dehydrating effect. This is certainly not a bad idea. It draws the attention to the molecular structures. They try to work it out on the blackboard:

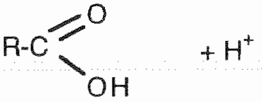
c6 No, but it works in any case as positive on the reaction. The *how*, that's the question.
c2 Ummm .. it splits like this ... [writes on the blackboard]:

$$H_2SO_4 \rightleftarrows HSO_4^- + H^+$$

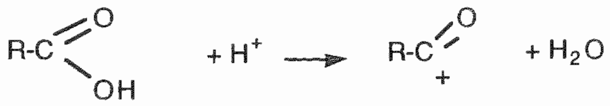
... and when you .. wait a moment .. that OH .. is that from alcohol?
c5 No. It's from the acid, I would think.
c4 It is the OH from acid with the H of alcohol.
c5 Yeah.

The students probably remember pieces of a mechanism taught in secondary school. At least one secondary school textbook mentions the mechanism of the Fischer esterification, but knowledge of this is not mandatory for National Assessment. Most students do not appear to know the mechanism. They continue:

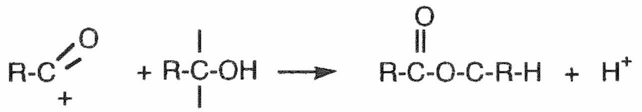
c2 Okay, then it is like this .. :



.. the H^+ .. so you get that .. umm .. yeah .. how that works I don't know exactly .. it's just an assumption .. for example that this .. [writes]



.. so this is a plus .. with that H_2O .. and that rest group .. reacts again with the alcohol .. [writes]



.. and that in turn results in .. an ester.

c1 Well no!

c6 You have that alcohol ..

c4 Now it cannot be explained why you all got ester without sulfuric acid.

c2 .. and there is an H^+ left..

c6 We're not dealing with that right now.

c2 .. and that H^+ with that H_2O .. gives that H_3O^+ ..

c6 Yeah .. but how do you deal with that plus charge on the carbon atom?

c2 That one .. it works like ah .. that's what is left over and this and that .. that's what you've got left and that works as a matter of fact .. that H_2SO_4 just signals the starting reaction .. to make ester.

c5 Yeah.

(...)

c4 But isn't that very illogical .. that would mean that an acid would react with an acid.

This last remark is very understandable from the point of view of the Brønsted theory. The proposed mechanism seems to violate one of the few theories the students can handle:

TA Wait a moment, somebody says: in this scheme, in the first step, an acid reacts with an acid.

c4 In that case that is what always should happen, an acid reacting with an acid, because there is nothing specific about the reacting acid that we have.

c5 But H_2SO_4 is a very strong acid, maybe that's got something to do with it.

c4 But .. have you ever heard or read that an acid can react with an acid?

c2 But you don't have water in your surroundings. You don't have H_3O^+ .. that is something completely different from what you get in secondary school.

c3 It is not a strong acid that formic acid, just acidic .. must become a base.

c2 You're dealing with 100% pure substances.

c6 But you would say .. that H^+ will rather react with that OH-minus .. or .. in any case with that OH-group .. and not with that acid-group. It is less attractive than that OH-group, in that case.

(...)

c1 It seems very unlikely to me

(...)

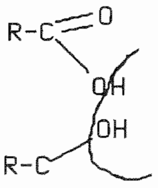
c4 Question: you assume that one acid reacts with another acid .. for that .. you might as well say that one carboxylic acid reacts with the other carboxylic acid ..

TA Yeah .. but sulfuric acid is a strong acid.

c4 Yes, yes, but you might as well say that sulfuric acid reacts with itself .. if acid reacts with acid.

The students continue debating this issue for a long time, with only occasional interruptions from the TA or from me. Two students, c4 and c1, try to refute the proposed action of the proton. c4, because she rules out the possibility of an acid reacting with another acid; c1, because he doesn't seem to believe that adding protons would change anything to the way esters are formed:

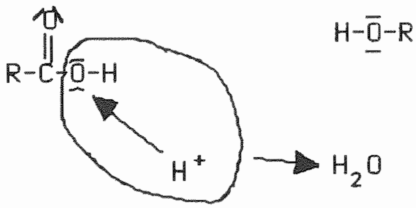
c1 I don't understand .. what are you doing .. why are we all of sudden bothering about H-plusses?
(...)
c1 Just look ... [walks to the blackboard and writes down]:



c2 Is that OH coming from the alcohol?
c1 That OH is split off and with this H it forms an H_2O molecule.
(...)
c1 And you got H_2O .. so H_2O .. well .. we started with .. with an acid and an alcohol. Well .. acid and alcohol .. and what do you got .. ester and water.
TA Yes, agree.
c1 Yes, well .. in this way you get it too. So why should it all of a sudden happen with H^+?
c2 Catalyst!
(..)
c1 The other scheme [points] is a detour. It is just a detour.
c2 But a catalyst *is* a detour!

In this second group discussion, the students did not reach an agreement. Their discussion reveals how difficult it is to develop structure-activity arguments when there is nobody present to tell 'how things really are'. The progression was not that they reached a chemically correct explanation, but that they made an issue of structure-activity-relations as such, and, in the same time, experienced the inability of the Brønsted theory to provide a convincing framework. In this discussion, the students finally gave up and just concluded that sulfuric acid seems to work. In the next group discussion, the issue was revisited:

c1 Did you ah .. by the way ... figure out .. how that worked with acetic acid? Why it was that that reaction went faster?
c5 Acetic acid faster?
c1 Yeah .. you know .. we had that big discussion on the blackboard and all that ...
c2 Yes!
TA Reaction mechanism?
c2 Never heard of it anymore.
c5 Oh ,with that reaction catalysis.
c1 Because I figured out something nice.
TA Well, go ahead.
c1 May I? [goes to the blackboard en writes:]



c3 Sulfuric acid.
c1 Sulfuric acid is added .. that is what it reacts with.
c3 Yes, okay.
c1 We just simply represent that with that H^+ .. and according to me this is electrophile and it also is..
c3 ..you heard that this morning! [refers to the lecture course on organic chemistry]
(laughter)
c2 Oh no, he told that two weeks ago, so ah ..
c1 Two weeks ago he said that .. look at this .. this forms water.
c3 This is exactly the same as last time!
c4 Exactly the same!
c1 No!
c3 Yes!
c1 Last time we reacted two acids with each other, so that was not correct.
c3 Yeah, but this is the same, isn't it?
c5 You also use two acids.
c1 No, not two acids.
c3 Yes you do.
c1 This is electrophile and nucleophile, that ..
c3 ..these are also two acids, that doesn't matter.
c1 Well! In any case I have said it this way.
c3 Yes okay, I see what you mean, but it does is exactly the same.
TA Yes, this is the same as last week.
c3 Exactly the same.
c1 Almost the same.
c5 Only with a different explanation.
c1 This explanation is different, more clear. That's the difference.

Although c1's explanation is not exactly more clear, it is different. The essential difference is the representation in the drawing of free electron pairs on oxygen. These were absent in the previous discussion. The use of the terms 'electrophilic' and 'nucleophilic' is appropriate in this context. Apparently, something the professor of organic chemistry told in his lectures struck a chord with c1 and made him apply these terms. However, he is completely laughed out of court by his fellow students. Even the TA joins in disapproval, presumably because c1 cannot clearly explicate his understanding.
In chemical terms, what is going on here is a shift from the Brønsted acid-base theory towards the Lewis theory. In the Lewis theory, an acid is an electron-pair acceptor, and a base is an electron-pair donor. A proton is an electron-pair acceptor whereas oxygen atoms have free electron-pairs to offer. So acetic acid can act as a Lewis base towards the proton. This theory thus demands a representation of structure that includes all electron pairs.

In hermeneutic terms, this is a case of a new issue coming into being, because a new viewpoint is discovered. From the point of view of the Brønsted theory, free electron-pairs do not exist. They are meaningless. All that is given are two acids: two proton-donors. These, as the students have learned, react with bases, not with each other. Hence, the statement 'acids do not react with acids' rules out any counter-example. All students, except c1, explicated their experiences with the phenomena under consideration from this point of view. The objects they saw and talked about were proton-donors. So nobody noticed the lines in c1's drawing representing the free electron-pairs. These have no meaning and thus could not be observed. From the point of view of c1, however, a different object is visible. To him, the free electron-pairs have become an issue. However, he was unable to find words that would draw the attention of the others to this issue. It seems that he could not understand why the others failed to see what was so obvious to him, but he could only point at it. An experience has led to the coming into being of a meaningful object for understanding. C1 was very sure of the correctness of his interpretation, but he was as yet unable to provide a rationale and to communicate his understanding in order to achieve common understanding. Intuitively, the student was applying the principle that an electron-pair donor and an electron-pair acceptor can react with each other, but he was not discussing his ideas in these terms. Instead, he used a fact-like language: "this is electrophile and nucleophile", whereas the other students preferred a different language: "these are two acids". In the absence of an explication of the terms 'acid' and 'nucleophile', the students did not approach each other.

The result of c1's efforts was in any case that attention was drawn once more to the interaction between the proton and the reactants. In his drawing, the proton attacks the acid and induces a splitting off of the OH-group. This was questioned:

c4 But why shouldn't that H^+ attack that OH of the acid .. no .. attack the alcohol?
c1 That's all right with me.
c2 That's also possible. If you like that better.
TA Ah, but what do you get in that case?
c2 The same, but reversed, you understand?
c1 Yeah, it doesn't matter from which one you take that OH.
c2 The only difference between alcohol and an acid is that in the one C a double O is attached, but ...
c4 But I have always learned that it is the OH of the alcohol .. ah ..
c1 No.
c4 ..the OH of the acid that splits off and the H of the alcohol.
c1 Yeah, but did they explain why that happened?
c4 No.

In this fragment, the students used terms that are compatible with the Brønsted context. Increasing attention was drawn to structural similarities and differences between alcohol and carboxylic acid, in order to explain chemical behavior. However, in the Brønsted context, there is no reason to differentiate between OH-groups. The students have knowledge nor understanding regarding the relations between acid or base strength and molecular structure.

In an intermezzo, the TA explains that chemists, by using acetic acid labelled with a radioactive oxygen isotope, have determined that the oxygen in water originates from acetic acid and not from alcohol. The students accepted this and continued:

TA So, that is an experimental fact.
c2 Yeah, okay.

c4 When you label this ..
TA If you label this one, then it is this O, okay?
c1 Well, that could have something to do with electronegativity, maybe.
c2 Yes, but ..
TA Yes, that is a difficult concept.

C1 once more introduces a term that belongs to the Lewis context, and he is not taken seriously again, it seems.

TA Well .. umm .. c1 .. why does that H just attack the acid, and not the alcohol?
c1 Yes, that ah .. oh ah .. look here ..
TA Yes, that has to do with electronegativity.
(laughter)
c1 If that O of that acid group is electronegative then it just attracts that H^+ towards it .. more than ah .. as .. of the alcohol .. if that is electro .. ah .. positive is.
c3 Yeah but an acid is never more electronegative, it is more electropositive.
c1 Yes.
c3 So it is more likely that he attacks the alcohol.
c1 No, especially if ah .. if the O of the acid group is more electronegative.
c3 Yes, *if*.
c1 Yes, if. Yes okay, I cannot say how it is .. I am just a freshman.
c4 But, question, okay. Now you are talking about that electronegative .. in that case that OH of that alcohol is more electronegative because it has 2 electrons of its own .. electron-pairs of its own .. plus 2 shared. And that other one suddenly has 3 pairs shared and 1 of its own. So that O should be more positive.
c1 No, no, no. That one also has 2, hasn't he?
c4 No, watch it. There with that OH of that acid .. of that alcohol, sorry .. it has 2 electron-pairs of its own, plus 2 shared.
c1 He has 2 unbound electron-pairs, yes.
c4 Okay, 2 unbound electron-pairs.
c1 Yes, no, I was not sure if we were saying the same thing.

C1 lacked a coherent framework and terminology to discuss the reaction consistently in the Lewis context. This context was not yet developed. The term 'electropositive' is not very productive, and his use of this term in this context sheds doubt upon his understanding of the term 'electronegative', too. He seemed to think that when a group attracts a positively charged proton, then it must be negatively charged itself: electronegative. When a group does not attract a proton, then it must be the reverse: electropositive. My interpretation is that students understand that full opposite charges attract each other, like they do in ions, but that they have difficulty applying the issues of charge distributions within a neutral molecule leading to the kind of localized partial charges that chemists indicate with $\delta+$ and $\delta-$.

Still, c1's perseverance brought another student (c4) to introduce into the discussion the term 'electron-pair'. C1 reacted as if it is obvious to discuss the issue using this term. Although he himself had not been very lucid he now wanted to be sure that they were talking about the same issue. He showed some awareness of the necessity to develop a shared language on the basis of a shared experience in this process of issuing discourse. However, it was just an incident. In general, the participants introduced and used terms without giving or asking an explanation of meaning. They continued (without break):

c4 And now all of a sudden that O would become more positive, in order to let that H^+ attack, and then he shares another electron-pair.
c1 Yes.
c4 So he has one less.
c1 Yes, then the product has already been formed.
c5 The C of that acid already was minus.
TA Well .. it is about this .. that H^+ .. it is here as a spectator, and it sees this one or that one. He sees both.
c4 Yes.
TA What does he go for. Is it possible to give a reason for that.
c4 That would .. in this case that would not give an argumentation .. it's all well .. just because we want to have that ester it is more convenient to draw it like that.
R There is yet another oxygen.
c5 Yeah, that one was already more delta plus than with the alcohol. Because that C was already more plus because of the other ..
c6 That double bonded O?
c1 May it also be double bonded?

Students have been exposed to chemistry professors talking about free electron-pairs, electronegativity, nucleophiles, and delta plus. During this ongoing discourse, however, they develop the understanding that these terms do not only appear on paper and in tests but also are applicable to their own experiences. Although in this discussion they seemed to be just guessing, they kept on trying:

c1 We will still be sitting here at 6 PM if we go on like this.
(laughter)
c4 But .. if you say .. that H^+ attacks that O .. why doesn't he attack that double bonded O?
c2 Because is it attached much stronger, that O.
c4 You say that that H^+ attacks that O.
c1 Yes.
c4 But it might as well be that double bonded O, it also has 2 empty electron-pairs.
c1 No, I don't think so.
TA Why not?
c4 That makes no sense!
c1 Because it is more electropositive.
c2 You should just look to the enthalpy of an..
c3 Yes! What about that? Do *you* know that?
(laughter)
c2 Well .. of a C double bound O with a C single bound O .. what the difference is .. to unbind that. The bonding enthalpy of those 2, that makes a difference.
c4 But you've got that H^+ .. you let that H^+ ..
c3 But that double bonded O has more electrons around it.
c4 H^+ attacks the free electron-pair of that O .. that other O also has 2 free electron-pairs.
c2 Yes, but you can't loosen those!
c4 Free electron-pairs are not fastened!
c2 But these are!
(laughter)

From a chemical point of view, the students did not proceed much. They were stuck with the first step: the addition of a proton to acetic acid. They did not proceed towards a discussion of the subsequent steps, let alone that they proceeded towards a complete mechanistic explanation of esterification. But from an educational point of view, they have started to apply structure-activity-relations. That implies that they have shifted to a

viewpoint from which objects belonging to an organic chemistry context have become visible and meaningful. Initially, students laughed about terms like nucleophile and electronegativity. These terms belonged to the context of the organic chemistry textbook with its paper and pencil question and exams. They seemed out of place when used to describe and interpret experiences, but this changed.
The relation between students' experiences and the jargon is an uneasy one, however. Since these terms are used in books and during lectures, students cannot deny that they are real and that there must be such a thing as electronegativity. They all know this, and, consequently, they overlook to ask each other what they mean when they use these terms. The students express themselves in a language that is not theirs. I think it would be better when students would first develop their own words to describe, say, why an oxygen atom in a neutral organic molecule could attract a proton. When an understanding of this issue is formulated, and the students are able to move around in the new Lewis context, their terms could be exchanged for those in use in chemistry. In this way, students would understand that electronegativity is an instrument for describing chemical properties, instead of knowing electronegativity as a fact.

During this lasting discourse, the students received little help from the TA or from me. We both were unprepared for this discussion. During long intervals we did not participate at all. This implies that the students saw enough reason to continue the discourse on their own, which is valuable. On the other hand, a teacher who would understand this process could be of tremendous help. Every few seconds misunderstandings occurred, and new terms were used without explanation. A teacher could structure the discourse, urge students to explicate themselves, point out inconsistencies, combine the results with other experiences, and, in general, organize a coherent and consistent discussion. In this discourse, the students could not resolve their impasse and turned to me to provide the 'correct' mechanism. This I did, since I thought they deserved to know after their effort. I pointed out that mechanisms are models meant to explain. They may also contain several more or less hypothetical transition states. I explained that the first step in this mechanism is an addition of the proton to the carbonyl oxygen. I used the terms 'electronegativity' and 'free electron-pair' to explain this. In a next step, I had water split off, and I draw attention to a full plus charge on the central carbon atom in acetic acid. Pointing at the free electron-pairs on the alcohol oxygen atom, I called this a nucleophile with respect to acetic acid, and continued with a final step in which the ester was formed and the catalytic proton was split off again. I also mentioned that this mechanism is called a nucleophilic substitution of the second order, a term the students had heard before, but which probably made sense to them at that moment. I finally told them that they could find this mechanism in their organic chemistry textbook (McMurry, 1988).
Whether this transfer of information was appropriate or not remained an open question, since I was not investigating these students' applications in a subsequent educational context. It seems to me that they now had acquired enough understanding of the chemical issues in this context to be able to understand new pieces of information in the same context transmitted to them in a lecture format.

From this analysis I drew the conclusion that it is possible to draw students' attention to structure-activity-relations through experiences in this educational context. I understood that part of the success was due to a coincidence: the mechanism of the catalyzed reaction is the same as the mechanism of the uncatalyzed reaction. Students' attention was drawn to the proton through a comparison between formic acid and acetic acid. The strongest acid proved to be the best in developing the ester smell. Their interpretation of the role of sulfuric acid could build on this experience. However, the rigid Brønsted context hampered progression. It was only after attention was drawn to the free electron-pairs on oxygen that a change towards the Lewis context could be made.

6.5 A sub-structure for structure-activity-relations

It now is possible to describe the elements of (molecular) structure that must be understood to be able to relate structure to activity. On the basis of previous work of De Vos (De Vos, 1990). it seems to me that chemical corpuscula represent chemical (re)activity with the qualities mass, space, energy, and time.

Mass

Element analysis of substances reveals two things: the identity of the elements present in organic compounds, and the relative mass proportions of these elements. For instance, the liquid ethanol is composed of 51.5% carbon, 35.1% oxygen, and 13.4% hydrogen. Using relative atomic weights this transforms to the empirical formula C_2H_6O. This formula simply represents the empirical facts deduced from combustion experiments. It does not literally say that ethanol contains two carbon atoms. It says nothing about structure; it is not even necessary to assume that ethanol is composed of a multitude of discontinuous particles. For that matter, it could have been one continuous piece of matter, consisting of chemical atoms. Vogelezang has described in detail the educational development of such formulae (Vogelezang, 1987; Vogelezang, 1990).

Space

However, there are several chemically different substances yielding the same empirical composition formula. For example, dimethyl ether has the same empirical formula as ethanol. On the other hand, there is only one reaction product with the formula CH_2Cl_2. Such empirical facts led Van 't Hoff and Le Bel to propose a tetrahedral three-dimensional structure around carbon to cope with this by representing these aspects in *space*. Molecular formulae resulted and were very successful. In the mean time, physicists had more or less agreed on the particulate nature of matter on the basis of physical experiments. Joling (Joling, Ten Voorde, & Verdonk, 1990) describes an interesting case of a discussion between the physicist Rutherford and the chemist Armstrong, taking place in the year 1914. The latter still adhered to the chemical atom (or molecule) as a theoretical principle representing chemical regularities Rutherford was unable to convince him that it is necessary to adopt the particle as a fact itself. The physical view eventually had the upper hand: in today's education, atoms are presented as facts.

It seems to me that the students described in this study have adopted this physical viewpoint. To them, molecules are particles consisting of atoms connected to each other in a spatial order. It is just one extra tacit step to assume that this model representation is an object that is subjected to the laws of classical mechanics. When a molecule is regarded as a physical object, it cannot at the same time be regarded as a model representing chemical regularities. From the viewpoint of mechanics, it is impossible to deduce the chemical differences between ethanol and dimethyl ether. Or, to understand why a proton would prefer an oxygen in acetic acid above an oxygen in ethanol. In mechanistic terms, all oxygen particles are the same. Hence, it is necessary to add another feature to the model.

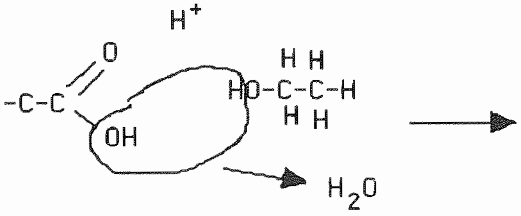
Energy/charge

By adding an internal *charge* distribution to atoms and molecules, potential differences can represent a wide variety of chemical reaction possibilities. It seems to me that the students in Esters 2 were developing an understanding of this feature. They experienced the lack of versatility of the mechanical representation and discovered the possibilities of an argumentation based on interactions between a charged proton and charges at oxygen. In this way, a chemical representation of bonding is developed to replace the physical, mechanistic one (Van Hoeve-Brouwer & De Vos, 1994). Charge distributions themselves are grounded on energetic states: each molecule tries to minimize its internal energy. This process can be represented by highlighting the charge distributions.
In Esters, the focus is on *localized* charges: a free electron-pair on oxygen, a charged proton, a charge surplus on the central carbon atom in acetic acid. These issues are represented by the Lewis formalism (Van Keulen & Verdonk, 1992). *Delocalized* effects could explain the chemical differences between ethanol and butanol, and between acetic acid and formic acid. The electron-donating inductive effect of the alkyl group in acetic acid destabilizes the carboxylate ion, and thus causes decreased acidity. For the same reason, butanol is a better nucleophile than ethanol. However, the discourse taking place in Esters showed no signs of attention for the issue from this point of view.

Time

A feature almost missing in the students' discussions in Esters is *time*. I already described that many students implicitly expect that the esterification reaction takes place instantaneously. Their experiences with the test tube experiments helped them understand that, on a macroscopic scale, reactions take time. A similar development seems necessary on the representational level. Although students proposed several ideas about the molecular transformation of acetic acid plus ethanol towards ester and water, they tried to do this in one step. There was no intention to represent the process in several subsequent steps in time. They apparently still needed to develop an understanding of the issue of transition state.
To illustrate this point I represent a fragment from the other group's discourse:

d2	Yes .. it has to be like this, according to me. The H of the alcohol reacts with that OH that is released and then .. then it goes .. that C-O double bond with that H of that catalyst get attached to that loose O of the alcohol. And then the H of the catalyst gets off again.
d1	Could you draw that please?
d2	[draws on blackboard:]



d2 ..and then this one gets loose and becomes H_2O .. and then ah .. and this O gets attached here .. if it's all right.

The tacit assumption underlying this scheme seems to be that it everything has to happen in one moment in time. Although this other group did not exactly duplicate the discussions in the first group–the quantity of the discussions related to structure-activity-relations was considerably less–their remarks had the same qualitative features, showing a similar state of understanding.

From these interpretations, several conclusions and consequences can be drawn. In the first place, the educational context of Esters 2 seems to be appropriate to develop an understanding of several structure-activity-relations, but the quality of this process could be greatly enhanced by more adequate teacher-guidance. Second, an elaboration of the educational context should check whether students are able to apply their understanding of localized charge effects to explain and predict chemical activity. Third, the new educational context should try to develop the understanding of the issues of delocalization and time. Fourth, an educational context could be created in which these new structure-activity-relations are developed in relation with new elements of reaction-type and synthesis-planning.

6.6 Simulation-of-research

The first time I explicated the issue of simulation-of-research was during the interpretation of Esters 2, when I was focusing on the discussion on equilibrium presented above that led to a hypothesis and a crucial experiment. I realized that the process of devising experiments on the basis of previous experience and argumentation lies at the heart of scientific research. At such moments, the groups acted like a research group. They listened to each other, set up a lasting discourse, and used each others findings.
Simulation-of-research functions as the theme that unifies the other issues. The reaction-type issue revolves around the determination of the mass balance, that is, the identity and relative amount of the substances present. These parameters are determined with the gas chromatograph. Knowledge of identity and relative amount can then be applied to synthesis-planning when students understand the function of measuring and calculation in experimenting. This would have been research-like if research in organic synthesis would be characterized by questions of yield and purity. However, synthesis should rather be regarded as a means to answer theoretical questions, such as explaining why, in the absence of a catalyst, formic acid reacts faster than acetic acid. *It is only through attention to structure-activity-relations that synthesis, as well as measuring, as well as calculation, as well as theory, can be combined and applied. All these activities together constitute a context of simulation-of-research.*

However, the activities of the students could not always be characterized as simulation-of-research. Too often, they were just interested in making the ester. I noticed that my design sometimes stood in the way. Although the educational context explicitly aimed at developing educational issues instead of chemical results, it still has a structure that is characterized by instructions, assignments, and a TA asking for results. In this context, students only accidentally propose hypotheses and experiments that are not directly helpful for making the product. Students had the freedom to elaborate their own ideas, but it would have been helpful if the TA's had been more able to guide such digressions.

I concluded that although the educational context seemed to produce the anticipated results, it was rather rigid. I noticed that I myself sometimes had enough flexibility to deviate from my own design, but my TA's had not. They wanted to execute the experiment according to the guidelines I gave them. If the TA's are to be able to supervise students setting up experiments that do not follow directly from the anticipated educational context, they need to have a broad experience with chemistry. This is not always guaranteed. On the contrary, the TA's did not derive their understanding of esterification from experience; crucial information was provided by my teacher manual. So they knew the correct chemical explanations and results, but they did not always knew the way to achieve this through experience and experiment. Since they were not always physically able to observe everything the students said and did, they sometimes missed the phenomena and experiences that sent students into reflection and discussion. In such cases the TA's had difficulty participating in the discussion, let alone supervising it.

However, I could not solve these problems because of lack of facilities for rigorous teacher preparation. Since Esters worked well in many respects, I decided not to greatly redesign it. Instead, I focused on an elaboration of the educational context. A new experiment should help students to enhance their understanding within a context that would be characterized by the simulation-of-research format, that is, without an organization depending on instructions. In the next chapter, I describe this new context.

6.7 Esters 3 and 4: reaching the level of saturation

The student manual of Esters 3 was in many respects the same as in Esters 2. I left out the assignments on washing with water. Instead, I added a row to the table of physical properties in which I copied the Handbook's remarks concerning the solubility in water. This row indicated that the solubility in water of sulfuric acid, acetic acid, methanol, ethanol, and methyl acetate is good; the solubility of 1-butanol and butyl acetate is low; and that ethyl acetate is slightly soluble. The teacher manual was revised to include advise to supervise a discussion on structure-activity-relations, especially with regard to the esterification mechanism.

The general pattern of events in Esters 3 closely resembled that of Esters 2. That is, a level of saturation was reached in my research on this educational context. I therefore restrict myself to describing the few new and worthwhile observations.

Simulation-of-research

The simulation-of-research format should enable students to pursue their own questions and hypotheses. An example of this was an experiment they conducted with iodine as a catalyst. On the basis of the test tube experiments, some students thought that iodine had an accelerating effect on the reaction. This led to some discussion, since most other students denied this. The others had not had the experience; moreover, they could not imagine the function of iodine in this reaction. As a result, one duo decided to try iodine, to compare the effects with using sulfuric acid. They discovered that the esterification reaction did take place in both cases, but use of iodine resulted in a lower yield than sulfuric acid:

h4 We had ah .. with iodine we have .. we made ethyl acetate and that did ah .. succeed rather well ..
(..)
h3 We had .. well .. 39% .. that was the last one .. yeah.
TA With? H_2SO_4?
h4 That is with iodine, iodine.
h3 With iodine.
TA There you got 39%?
h3 That is not really much.
h2 That's low!

This disappointing conclusion was reinforced by a short discussion on structure-activity-relations. Nobody was able to suggest a convincing rationale for the catalytic function of iodine, so they concluded that after all it did not really have an effect. From a short-term chemical point of view, using iodine in this way was futile. From the simulation-of-research point of view, I however appreciated this very much. It is a case in which a tentative hypothesis, based on an experience, is followed by a controlled experiment. Since the a priori argumentation regarding the role of iodine as a catalyst was inconclusive, it was very appropriate to experiment.

Another case in which the simulation-of-research format proved appropriate concerned the assignments I had included in Esters 1 and 2 meant to draw students' attention to washing with water. In Esters 3 these tasks were left out, and they were indeed not necessary. The students used the table of properties and had no difficulty proposing washing with water:

h1 Ah .. ethyl acetate .. there is ah .. methanol still .. acetic acid .. and iodine.
TA And iodine.
h1 Yes.
TA All right. How do you think to ..
h6 You also have water in it.
h1 Yeah, okay, you also got a percentage of water in it.
TA Yes?
h1 Yes.
TA Okay. How ah .. are you going to get rid of all that?
h1 Ah .. ethanol .. washing.
TA Washing.
h1 Washing with water seems most logical to me. It has low .. it does have low solubility.
h5 Solve it in water?
h1 With a separatory funnel.

On the basis of the chromatographic analysis of the crude synthesis samples, it became clear that the students who used excess acetic acid had the highest ester to alcohol ratio. This was discussed explicitly in the context of the purification plans, and another student suggested to apply this idea. They compared the proposal with direct purification:

h3 What we also can do is add much more acetic acid than we had .. so that simply .. no .. ah .. no butanol .. ah .. ethanol would remain.
h7 Well, yeah ..
h8 Good idea.
h1 You could react it again with acetic acid, but I am not sure whether that is profitable.
h2 Yeah .. when you go distilling you'd better start distilling right away now.

h1 Yeah ..if you would .. like them .. add much more acetic acid to .. get rid of the ethanol .. you might as well start all over again.

Thus, the two students (h3 and h4) decided not to add extra acid but to extract and distil. This, however, did not lead to satisfying results. After this experience, they finally added extra acetic acid to the crude product:

TA You were thinking about acetic acid, weren't you?
g3 Yeah .. we finally did that .. with the butyl ester. In order to get rid of the butanol.
TA Yes.
g4 To make it really pure.
g6 So you actually did the same as them, only afterwards?
g4 Yeah, actually we did, yes.
g2 That's not exactly the fast way.
g6 Yes .. no.
g4 No .. it had to reflux again, actually.
g2 Yes.
g4 Well .. we had it reflux a little bit during the last distillation, that's what we did.
TA You could have thought about that before.
g4 Yes, indeed. But then we didn't know that it would cause problems .. that it would be so difficult to purify.

This illustrates that there is an *educational order in synthesis-planning*. Students are willing to use an excess amount of a starting reagent, but only when more straightforward purification techniques fail. They first have to understand the difficulties with purification before they relate purification with formation.

In Esters 4, I again added some minor improvements to the manual. The main reason for conducting Esters 3 and 4 was not to gather more data on students' understanding. Instead, Esters became a preparation for a second cycle within the educational context. I designed an expansion, called Ethers, which built on students' previous understanding, and aimed at elaborating their understanding in the ways indicated in this chapter. I will report on Ethers in the next chapter. In Esters 4, I also focused on the teacher's cycle. I will describe my experiences with this in the last, concluding chapter.

7 Application

7.1 Ethers 1

Esters has prepared the students for an extension of the educational context that is to take place in a subsequent cycle, called *Ethers*. The students' cycle becomes a spiral: students are supposed to be able to apply their understanding in an expanded context. In this section I first summarize the findings of Esters, and the consequences this has for the expanded educational context.

From the point of view of *synthesis-planning*, Esters enables students to understand the issue of planning as such. More specifically, it should help them to consider the analysis of the mass balance and to relate the purification stage to the formation stage.

From the point of view of the *reaction-type*, Esters develops the notion of the equilibrium reaction with a side product: $A + B \rightleftarrows C + D$. This understanding is applicable in synthesis-planning: a better result can be achieved by using an excess of a starting reagent and/or by removing one of the products.

From the point of view of *structure-activity-relations*, the very idea of a molecular structure representing chemical activity is developed. Students acquire some understanding of the way localized charges can provide rationales for organic chemical reactions. Structure-activity-relations can explain why a certain mass balance (and hence, a certain reaction-type) occurs. This understanding can be applied in synthesis-planning, since it suggests criteria to be met by the starting reagents. For instance, if students had already understood structure from the viewpoint of localized charge, they could have understood the chemical notions of leaving group and nucleophility and hence, they could have understood the applicability of acid anhydride in making esters. Their experiences with Esters helped them to develop the necessary understanding of the Lewis representation, which I think they can apply now.

If students have understood these notions to a certain extent, they must be able to apply this understanding. The consistent way to investigate this is to bring them into a new educational context that elaborates on the same issues. This is done in Ethers, which takes place some three to four months after the completion of Esters. By that time, the students also have completed the first year lecture course on organic chemistry. In the schedule of the laboratory course M&M1, Ethers took the place of the second organic synthesis, which was a classical prescription experiment on making bromohalides and chlorohalides from alcohols. Ethers 1 was done by four groups of eight students. Two groups (g and h) previously had done Esters 3; the other two groups (e and f) had not.

In Ethers, I tried to apply the *simulation-of-research* format more rigorously than in Esters. In order to get started, the students initially are confronted with a similar question as in Esters: How would you prepare ethers? But it is made clear from the start that this synthesis is a pretext for investigating the process as such, from whatever viewpoint the students think would be appropriate. This implied that there could be no prescribed assignments or activities. The experiments should be based on discussions, hypotheses, experiences and argumentations.

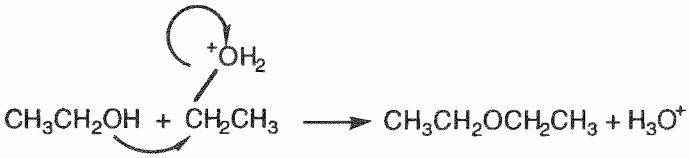
Students have no secondary school knowledge of the synthesis of ethers, however, it was a topic in the lecture course on organic chemistry. The course and the textbook mention several methods of preparing ethers. One of the most versatile methods described was developed by Williamson in the middle of the nineteenth century and consists of the reaction between an alkyl halide (R_1X) with a sodium or potassium alkoxide ($NaOR_2$) [McMurry, 1988 #131], pp. 622-625). Since then it is called the *Williamson ether synthesis*. I choose this synthesis to build the educational context of Ethers, because it has the potential to draw attention to a new reaction-type and to a new structure-activity-relation.

7.2 The student manual of Ethers

A week before Ethers was scheduled in the laboratory course, the students received the student manual. They were asked to read the text, answer the questions, and prepare for the pre-lab discussion. The (complete) text was as follows:

ETHERS

Industrially, *ethers* are often prepared with the so-called sulfuric acid method*. In this method, an alcohol is heated in the presence of concentrated sulfuric acid. In this process, water is generated too. The reaction probably occurs through a protonation by sulfuric acid of the oxygen atom in the alcohol molecule. Another alcohol molecule then substitutes water. In this way, diethyl ether is prepared from ethanol:



$$CH_3CH_2OH + \overset{^{+}OH_2}{CH_2CH_3} \longrightarrow CH_3CH_2OCH_2CH_3 + H_3O^+$$

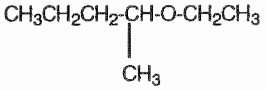
However, this method is seldom used to synthesize so-called *unsymmetrical* ethers. Unsymmetrical ethers are ethers that have two different groups attached to the central oxygen atom. An example is ethyl-pentyl-ether.

Question 1: What could be the reason for this? What would happen if you would heat a mixture of ethanol and pentanol in this way?

In this experiment we will concentrate on the following three unsymmetrical ethers:

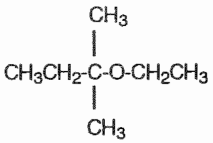
$CH_3CH_2CH_2CH_2CH_2\text{-}O\text{-}CH_2CH_3$

n-pentyl-ethyl-ether



$$CH_3CH_2CH_2\text{-}\underset{\displaystyle CH_3}{\underset{|}{C}}H\text{-}O\text{-}CH_2CH_3$$

sec-pentyl-ethyl-ether



$$CH_3CH_2\text{-}\overset{\displaystyle CH_3}{\overset{|}{\underset{\displaystyle CH_3}{\underset{|}{C}}}}\text{-}O\text{-}CH_2CH_3$$

tert-pentyl-ethyl-ether

This experiment has three objectives. (1) We will try to develop a workable procedure for the synthesis of unsymmetrical ethers that can serve as an alternative to the sulfuric acid method. (2) We will try to actually synthesize these ethers. (3) At the same time, it is the intention that you understand the new procedure and are able to provide an explanation.

So, we are looking for an alternative for the sulfuric acid method. There are two different approaches: (1) to start with the same starting reagents, but apply different conditions; (2) to use other starting reagents.

Question 2: Can you think of different conditions in which it is possible to use the same starting reagents?

Question 3: With which other starting reagents could you also synthesize these ethers?

Perhaps you consider this a difficult question. In that case you could get some help from a theory called *retro synthesis*. Retro synthesis is a kind of thought experiment in which your starting point is the molecule you want to make. You divide the molecule into two parts; from these parts you construct two starting reagents that, together, would combine to form an ether.

Question 4: What would be a suitable place to divide the ether molecule?

Dividing a molecule into two implies the breaking of a bond. Such a bond represents an electron pair.

Question 5: How will these electrons be divided over the parts?

You now have two parts. Now you have to assemble these into complete molecules again by attaching an extra atom (or a group of atoms, say, a functional group). It is wise to choose groups that can be released as easily as possible during the reaction. Otherwise you run the risk that the two substances do not react with each other at all.

Question 6: According to you, which groups can be considered for each part? Why?

You now have selected several starting reagents. But that is not a complete synthesis. An organic synthesis can be seen as consisting of several steps in which you go from starting reagents to the product.

Question 7: Which steps do you have to take with your starting reagents to produce a pure end product?

Write down your answers in your lab note book. During the pre-lab discussion we will decide together which procedures and which starting reagents we actually will investigate. This is still open; it depends to a great deal upon your choices. Other conditions are the availability of substances and equipment, and safety. It is intended that the various possibilities will be divided among the members of the group, so we can investigate various aspects of the synthesis.

Halfway we again will have a group discussion, to discuss the provisional results and problems, and to decide how we will continue. When the experiment is over we will determine the final results in a last group discussion.

*) See McMurry, second edition, page 622.

7.3 A justification of the educational context of Ethers

In Ethers I tried to amplify students' understanding to include the *side-reaction* as an extension of the issue of reaction-type. This was combined with an attempt to extend their understanding of structure-activity-relations towards the issue of *delocalization*. This elaboration took place in a simulation-of-research context of planning and investigating synthesis procedures for making ethers. In this section I explain my intentions and expectations in more detail.

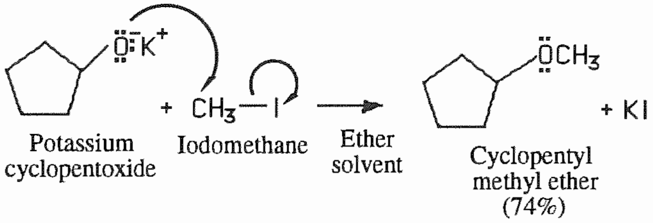
The student manual set an agenda for experimental work without much guidelines. It was intended that during the pre-lab discussion the students and the TA will discuss plans and ideas concerning the problem. The only constraints were those mentioned in the student manual, plus a time constraint: the experiment was to be completed within three four-hour lab periods. When the experimental work would be finished the students were to write a report, the details of which would be decided upon during the last group discussion.

During the TA preparation, I discussed the simulation-of-research format of this experiment. The role of the TA was to elicit ideas, opinions, and hypotheses from students and discuss these with the whole group. The TA would assume the role of an experienced chemist who unfortunately does not know how to make ethers either, but who otherwise possesses enough knowledge of substances, equipment, and techniques to give practical advise. I realized that the TA had a difficult role to play. I expected them to be able by themselves to lead discussions and to have enough chemical and research experience to help the students with their experimental work, since I could not develop these qualities through teacher training.

I anticipated that the students would have read the text of the student manual and tried hard enough to answer the questions to make a group discussion meaningful. It is expected that students initially take the viewpoint that synthesis is about making products. Thus, they would reject the sulfuric acid method as inefficient, for this method will also lead to diethyl ether and dipentyl ether. If they would follow the student manual, they would have to conjecture other starting reagents with the aid of the retrosynthetical method. I anticipated that they would divide the ether molecule at oxygen and allot the electrons to the oxygen atom. That would yield the fragments RO^- and R^+. These fragments are both 'ionic'; they carry a full, localized charge. Students understand the structure-activity-relation that is represented by ions: it represents the potential for the simple reaction-type $A+B \rightarrow C$. Esters had made students aware of by-products. I explicitly draw their attention to this issue by focusing on the functional groups that have to be attached to the fragments.
The topic 'leaving group' is dealt with explicitly in the lecture course, so it is within students' reach to think of attaching an iodine or bromine ion to the alkyl fragment. They have been informed about what are 'good leaving groups', although they probably do not yet understand the underlying rationales. I thought it less probable that they would attach an alkali ion to oxygen. Alkali metals are in general categorized by students as inorganic and not as being a part of organic substances. They probably would suggest hydrogen instead, thus turning the fragment into an alcohol. They had experienced the nucleophilic properties of alcohol in Esters, in which context attention was drawn to the localized charges on oxygen. So they probably would settle for the alcohol. In a simulation-of-research context, this suggestion could serve as a starting hypothesis equally well.
By having students decide upon their starting reagents, I elaborated on De Jager, who thought that students cannot choose this. In my opinion, the retrosynthetical approach gives students the opportunity to apply those structure-activity-relations they already understand. Students are prepared for this free orientation by their previous experiences in Esters.

However, I anticipated that many students would instead use their textbook to elicit ideas, especially since I referred explicitly to McMurry. The Williamson method is described as follows:

> Metal alkoxides react with primary alkyl halides and tosylates by an S_N2 pathway to yield ethers, a process known as the Williamson ether synthesis. Discovered in 1850, the Williamson synthesis is still the best method for the preparation of ethers, both symmetrical and unsymmetrical.



> The alkoxide ions needed in the Williamson reaction are normally prepared by reaction of an alcohol with a strong base such as sodium hydride, NaH (section 17.4). An acid-base reaction occurs between the alcohol and sodium hydride to generate the sodium salt of the alcohol:
>
> $$\text{R-O-H} + \text{NaH} \longrightarrow \text{R-O}^- \text{Na}^+ + \text{H}_2$$

McMurry also mentions an esoteric looking method known as alkoxymercuration:

> A[n] (..) **alkoxymercuration** reaction occurs when an alkene is treated with an *alcohol* in the presence of mercuric acetate (mercuric trifluoroacetate, $Hg(OOCCF_3)_2$, works even better). Sodium borohydride-induced demercuration then yields an ether.

I expected students to prefer the Williamson method because it promises success ("still the best method") and seems to be a simple, direct process, whereas the other method uses a compound that probably is highly toxic (the mercury acetate) and applies unknown processes with difficult names ("sodium borohydride-induced demercuration").

Alcohols too appear in a variation of the Williamson method mentioned by McMurry:

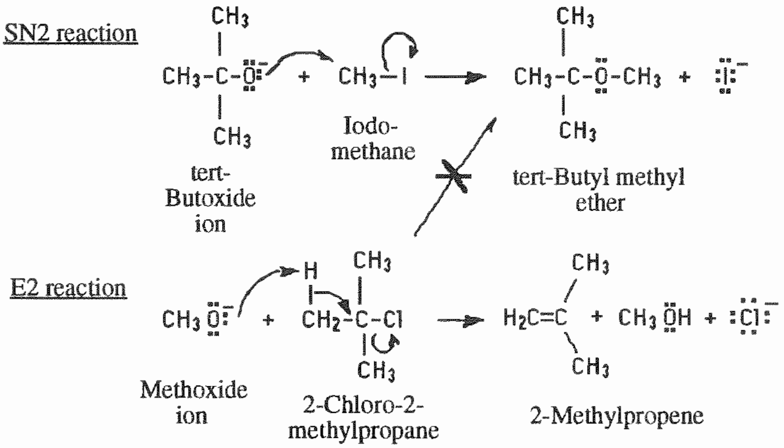
> An important variation of the Williamson synthesis involves the use of silver oxide, Ag_2O, as base, rather than NaH. Under these conditions, the free alcohol reacts directly with alkyl halide, and there is no need to preform the metal alkoxide salt. For example, glucose reacts with iodomethane in the presence of Ag_2O to generate a pentaether in 85% yield.

I expected that students would feel attracted to this method, since it appears to be very easy.
I made sure that a great variety of chemicals was in stock. Although McMurry's example shows an iodine compound, I choose bromine, mainly for reasons of safety. Alkyl iodine compounds are more harmful than are the corresponding bromine compounds. Present were bromoethane, *n*-bromopentane, *sec*-bromopentane, and *tert*-bromopentane. I also made sure silver oxide was in stock. The laboratory was well-stocked with other common organic reagents and solvents, so students could use many other substances too.
Instead of pure potassium or sodium hydride I had pure sodium in stock for the preparation of alkoxides. My personal experiences with using commercially available solid sodium ethoxide were disappointing, so I decided to have students prepare sodium ethoxide *in situ* from sodium and absolute ethanol, if they wanted to use this substance. I myself prepared in advance solutions of sodium *n*-pentoxide in *n*-pentanol, sodium *sec*-pentoxide in *sec*-pentanol, and sodium *tert*-pentoxide in *tert*-pentanol from the reactions between sodium and the alcohol. These preparations unfortunately are too slow to include

into the students' laboratory hours. Also present were the alcohols ethanol (absolute), *n*-pentanol, *sec*-pentanol, and *tert*-pentanol.

Ethers 1 was not meant to be a form of discovery learning. Students were not supposed to rediscover the Williamson method. Instead, the objective was that they expand their understanding of reaction-type, synthesis-planning, and structure-activity-relations in a simulation-of-research format. So it is not crucial whether their starting reagents are inspired by literature or by retro-synthesis. What matters is their argumentation. Now there is a caveat in making ethers with the Williamson procedure. The method uses an alkali alkoxide as reactant. It is known that these reagents can also react as strong bases. They can react with alkyl halides in an elimination reaction, leading to an alcohol, a metal halide, and an alkene. This typically depends upon several conditions. McMurry explicitly mentions this issue on the same page (p. 623):

> Mechanistically, the Williamson synthesis is simply an S_N2 displacement of halide ion by an alkoxide ion nucleophile. The Williamson synthesis is thus subject to all of the normal constraints on S_N2 reactions discussed previously (Section 11.5). Primary halides and tosylates work best, since competitive E2 elimination of HX can occur with more hindered substrates. For this reason, unsymmetrical ethers should be synthesized by reaction between the more hindered alkoxide partner and the less hindered halide partner, rather than vice versa. For example, tert-butyl methyl ether is best prepared by reaction of tert-butoxide ion with iodomethane, rather than by reaction of methoxide ion with 2-chloro-s-methylpropane:



Section 11.5, like the section on ethers, is dealt with in the lecture course. However, on the basis of Esters, my hypothesis is, that, for two reasons, the students, still are unable to understand what they read in McMurry with respect to elimination. First, they have not yet developed an *applicable* understanding of the side-reaction. Students will have attention only for what they consider to be the main reaction: the substitution reaction in which the ethyl-pentyl-ethers are formed. They will have no attention for the side-reaction in which pentenes are formed. Second, they are not yet able to understand the mechanism of the elimination reaction. The students have to compare a reaction that involves a nucleophilic interaction between two atoms both carrying localized net charge with a reaction that

involves an atom which propensity towards interaction is influenced by the rest of the molecule. In elimination, a strong Lewis base, carrying localized net charge, attacks a proton that seemingly does not carry any specific charge. The acidity of these protons is increased because the methyl groups in the β-position stabilize an incipient negative charge. The students have yet to learn to see a molecular structure as representing such delocalized effects. At present, none of the protons will appear to them to be acidic.
The students should be able by now to understand the nucleophilic substitution reaction, since Esters made explicit how localized charges in molecular representations can be related to chemical reactivity. I have chosen the Williamson ether synthesis because it draws attention to structure as a representation of delocalization, and at the same time draws attention to a new reaction-type.
Steric hindrance, which is used by McMurry to explain the predominance of second order elimination (E2) over second order nucleophilic substitution (S_N2) in the case of tertiary substrates, is a spatial representation of low reactivity, and could be understood by students. However, low reactivity towards nucleophilic substitution is not the same as high (or even considerable) reactivity towards elimination. Steric hindrance, as a spatial representation, does not represent the phenomenon of elimination. To understand why elimination occurs at all, and to compare first or second order elimination with first order substitution, a representation of the issue of delocalization has to be developed. What is needed is a representation of the stability of the carbocation or the transition state, which shows that some positive charge is allotted to certain protons. It is out of students' reach to judge the relative disposition of a molecule or a carbocation towards elimination and substitution. The empirical fact that 'more hindered substrates' are liable to elimination can be transferred to students as a piece of information, but that does not necessarily lead to an applicable understanding.
Thus, my hypothesis is that students do not yet have the understanding that would allow them to apply McMurry's information, even if they know it. I predicted that they therefore would not use this information. The practical consequence of this is that, when they would opt for the Williamson method, they would not be able to convince themselves that it would be wrong to start with ethoxide and *tert*-bromopentane. It is my intention that the educational context of Ethers would develop this understanding. The improved understanding of structure-activity-relations could then help to provide a rationale for the occurrence of the new reaction-type. This understanding, in turn, can be applied in synthesis-planning to prevent or investigate the issue of elimination.

The reason for choosing the pentyl compounds and not, say, the butyl compounds lies in the fact that a detectable side-product has to come into being, to be able draw attention to the issue of the side-reaction. Pentenes are liquids at room temperature, whereas the butenes are gaseous. An elimination reaction producing butene would go unnoticed by the students, since they do not have attention for this product. It will escape as a gas when it is formed. Pentenes will remain in the reaction mixture and can be detected as an extra constituent. Gas chromatographic analysis of certain crude reaction mixtures will reveal the presence of too many substances, begging for an interpretation.

I expected that the students have developed an understanding of synthesis-planning and that they will apply this by taking into account possible purification problems when designing the formation stage. In this experiment, they have several opportunities to apply this understanding. For instance, from the purification point of view it is better to start with *n*-bromopentane and sodium ethoxide in ethanol than it is to start with bromoethane and sodium-*n*-pentoxide in *n*-pentanol, since it is much easier to get rid of the ethanol than it is to get rid of the pentanol. It is also wise to use a little sodium ethoxide in excess, to make sure that all the bromopentane is used, since this substance has similar physical properties as the resulting ether. On the other hand, it is also difficult to extract *tert*-pentyl-ethyl ether from a *tert*-pentanol solvent, since these liquids have comparable physical properties. This would suggest to start with *tert*-bromopentane. However, this would lead to even greater problems, due to elimination taking place. Here, students have an opportunity to compare purification problems with reaction-type problems, or, in other words, to compare purity with yield. Since I expect them to have little attention for the elimination, their current understanding of synthesis-planning could suggest them to start with *tert*-bromopentane.

In Esters, the students have learned that it is important to analyze samples of reaction and purification mixtures to determine the result of a certain action. It is expected that they will do so in Ethers right from the start. In Esters, gas chromatography proved a versatile method and it is expected that they will apply this method again. In Esters, the end products themselves were available. The reaction samples could therefore be compared with the pure esters. This is not possible in Ethers: I did not provide the pure products. My aim was to expand students' understanding of characterization in this way, since it now becomes necessary to identify unknown constituents. I hoped that the experience of unidentified GC peaks would induce a wish to apply identification techniques. In the process of identifying an unknown constituent expected to be the ether, students could in this way stumble upon the pentenes.

From a chemical point of view, there are various possibilities to identify the products. The metal halide that is formed will be insoluble in most organic solvents and is, as a precipitate, easily recognized. The presence of ethers can be detected with infrared spectroscopy, even in a crude mixture, since these ethers have a strong characteristic absorption at about 1120 cm^{-1}. Alkenes also have characteristic infrared absorptions. They also can be detected in other ways, for instance through their ability to decolorize a bromine solution and through their UV-absorption. However, to characterize pentenes in this way, students would already have to have a specific expectation. An excellent generic technique would be GC-MS. Gas chromatography would give information on the number and relative occurrence of the substances in a sample, whereas mass spectroscopy would give the information from which these substances could be identified. However, the students do not yet know or understand mass spectroscopy. The same holds for NMR. Students would have to rely on the interpretation of experts. Interpretation of infrared spectra is less complicated, since peaks on a spectrum can be directly correlated with functional groups in a molecule.

Thus, I concluded that gas chromatography and infrared would fit in best in this educational context. They offer the necessary information in forms that can be interpreted by students. If they would have made pentenes, they would be able to tell by themselves with the help of IR.

I anticipated that students would pay attention to the chemical results in terms of yield. They can compare different routes toward the same product. They, I expect, will notice that a high yield only is achieved if a primary alkyl halide had been used. On the basis of empirical experiences attention is drawn to the structural differences of primary, secondary and tertiary compounds to explain differences. In this way, an analysis of mass balance (synthesis-planning) leads to the discovery of the side-reaction (reaction-type), and this, I hope, helps to expand students' understanding of structure-activity-relations towards delocalized stabilizing and destabilizing effects. For this, it necessary that they will ask themselves theoretical questions. The simulation-of-research format should help them not to focus exclusively on making ethers.

The educational context hardly contains any directions or assignments. It is expected that students will show improved ability to pose and investigate their own questions, under the supervision of the TA. The TA is expected to make sure that each student conducts experiments that will help to answer the general questions on the process to make these ethers. Students should not all do the same things; as a group they should cover several alternatives to make comparison possible, and focus on various questions and hypotheses. The experiments the students can do are of course constrained by matters of safety, the availability of reagents and equipment, and the time allotted for this experiment (three four-hour periods).

For efficiency's sake I had made a list of the physical properties of the substances that I anticipated could be proposed by the students. The *Handbook of Chemistry and Physics* (Weast, 1989) uses systematic names, which makes it rather time-consuming to find the substances under consideration, especially to students who are neither accustomed to the IUPAC formalism nor to the Handbook itself. From my list, the TA could copy the properties of those substances that actually were used by the students and hand out the copy. The list contained molecular weights, boiling points, densities, refraction indices, and solubility properties of the three ethyl-pentyl ethers, the four alcohols, and the four bromoalkanes, but not the properties of the alkenes.

The boiling points are: ethyl-*n*-pentyl ether 120°C; *n*-bromopentane 130°C; *n*-pentanol 137°C; ethyl-*sec*-pentyl ether 109°C; *sec*-bromopentane 117°C; *sec*-pentanol 119°C; ethyl-*tert*-pentyl ether 101°C; *tert*-bromopentane 108°C; *tert*-pentanol 102°C; ethanol 79°C; bromoethane 38°C. For someone understanding synthesis-planning it can be concluded that it is undesirable to end up with crude mixtures containing both the ether and the bromopentane or the pentanol, especially since the solubility properties of these substances also are comparable.

I anticipated that students would want to use gas chromatography for the analysis of samples. In order to save time, I prepared reference chromatograms of all the organic liquid starting reagents and solvents. I used a column temperature of 80°C and columns with a polar stationary phase (CP-SIL88) and an apolar phase (OV101). Copies of these chromatograms were made available to the students through their TA. The chief difference between polar and apolar chromatograms is the position of ethanol. In the apolar chromatograms, ethanol has a short retention time, whereas it is retarded more in the polar column. By comparing the two, it becomes visible whether or not the ethanol peak covers another peak.

For the reader's sake, I describe in advance the composition of typical chromatograms. Many students used starting solutions of either sodium ethoxide in ethanol with bromopentane or sodium pentoxide in pentanol with bromoethane. The first kind of mixtures yielded (apolar) chromatograms in which ethanol appeared first, closely followed by the elimination product pentene (if present). Next came the ether, and lastly the bromopentane. The second approach yielded chromatograms in which bromoethane appeared first, followed by the ether and a broad peak of the pentanol solvent.

7.4 A description of actions and events

Ethers 1 elaborates on Esters 3, and this proved to be disadvantageous for the groups that had not been involved in Esters. It appeared that the three lab periods were barely sufficient for the two groups with Ester experience to complete their attempts. The other two groups had some problems to get started. After four months of prescription lab they had difficulty with the simulation-of-research format, continually expecting to be told what to do. They also were slower to pick up gas chromatographic analysis, since they had not used this technique in as a tool for analysis in organic synthesis before. As a result, their experimenting had to be ended before purification and analysis were completed for all students. This was not the case for the Ester groups.

All groups started with a group discussion. The first theme was the sulfuric acid method. As expected, students rejected this method because of its low theoretical yield. In discussing alternatives, it soon became apparent that many students had read McMurry's section on ethers during their preparation. Hence, they favored the Williamson method, including the silver oxide variation, whereas they rejected the mercury alternative. During the discussions, it became clear that many students had read the sentences on elimination. Some students explicitly brought up this issue, stating that it is undesirable to start with the "more hindered halide partner". However, it also became apparent that they did not really understand why. Eventually, all kinds of combinations of starting reagents were chosen, including those disfavored by McMurry. Students supposed that these reactions would be slower because of the steric hindrance. In a simulation-of-research, they set out to check this hypothesis.

The students in general assembled a reflux apparatus and regularly took samples for gas chromatographic analysis. Those students who previously had done Esters did indeed look for possible purification problems. Some started with a small excess of ethoxide to make sure that no bromopentane would be present after completion; others chose an excess of bromoethane in order to use up all sodium pentoxide.

All reactions involving sodium alkoxide showed a reaction phenomenon in the form of the precipitation of a white-yellow salt. The students had no difficulty identifying this precipitate as NaBr. Students starting with a combination of alcohol, bromoalkane, and silver oxide in general saw nothing happen. This was confirmed by analysis. One student, for reasons to be discussed below, added KOH to his mixture of ethanol, *n*-bromopentane, and silver oxide. As a result, a salt precipitated, gas chromatography revealed the formation of a new product, and the flask became coated with a silver mirror. Apparently, silver oxide was reduced, but it is not clear which reductor caused this phenomenon.

During GC analysis, it became apparent that several students had a peak too many. Although the issue of elimination had been discussed explicitly during the preliminary group discussion, there was not one student who linked the appearance of this extra peak to the formation of a pentene.

Students applied several purification strategies: filtration, washing with water, extraction with diethyl ether or hexane, and/or distillation. One student, stuck with *tert*-pentanol as a solvent, decided to remove this by repeated reaction with sodium and distillation, in a procedure remarkably similar of one mentioned by Vogel. Not all students succeeded in isolating their product; especially those whose main product in fact was a pentene instead of the ether they expected. With infrared spectroscopy, students in general were able to identify the presence or absence of ether in their samples, but they were not able to identify the pentene. It appeared that the ethers had a characteristic, rather sweet smell, whereas the pentenes, as a chemist would expect, smelled awful. Students noticed this smell too, but could not identify it.

Eventually, students concluded that it is wise to start this synthesis with unsubstituted bromoalkanes, not because steric hindrance slows down the reaction, but because no ethers are formed the other way round. They also concluded that the silver oxide method in general did not work, but they were unable to find reasons for this.

7.5 Synthesis-planning

With respect to synthesis-planning, I was interested in whether the students would apply their understanding acquired in Esters, and whether they would develop an understanding of structure-activity-relations to account for and prevent side-reactions caused by reagents with high reactivity and low selectivity.

The first aspect especially applies to relating the purification stage to the formation stage and to the analysis of the mass balance. For those groups not involved in Esters, figuring out things like taking and analyzing sample took a lot of time, and they initially had more difficulty interpreting the chromatograms. The Ester groups did not have these difficulties, since the activities were approximately the same as in Esters. To them, it was a matter of routine to run a chromatogram at relevant times.

More interesting were the decisions regarding the formation stage. The students who had not participated in Esters in general started with the exact molecular stoichiometry. Some started with a small excess of bromoalkane, because in this way they hoped to prevent the sulfuric acid reaction, that is, a reaction of the alkoxide with the solvent alcohol to form a symmetrical ether:

e1	You have to make sure that you cannot have an excess of that ah .. sodium thing .. because when it is gone, that bromopentane .. ah .. then ah .. that OH will react further.
e7	Yeah.
TA	Yes. Yes. So you say: I take 100% of this and 100% of that .. because .. when this is gone, then that will be gone too, and this cannot happen any more?
e1	Yes.
e7	Well .. maybe .. ammm ..
e1	Yes I think that, yes. Or maybe an excess of that ah .. bromide .. so that you are sure that the other not ah .. reacts.
e7	Yes.
e1	Yeah, that's what I think. Even an excess of that ah .. bromopentane.
e7	Yeah because .. yeah.
e1	101% excess.

As a consequence, the students making *n*-pentyl-ethyl ether did succeed in making the ether but got stuck with some bromopentane in their crude products.
The Ester groups, on the other hand, showed the expected understanding of synthesis-planning by taking a reasoned excess of the substance that would be the least difficult to remove afterwards:

TA	And, g4, what are you going to do?
g4	Well, I thought about taking a little bit less of the pentoxide.
TA	Because?
g4	Because with distillation it is very easy to remove that little alkyl halide. So .. in case of purification.
TA	Is it so easy to remove, that alkyl halide?
g4	I really think so, I think the boiling point of it is much lower .. than that of the tertiary alcohol. (..)
g3	Yeah, me too, I wanted to take a little bit more of that ethyl bromide. (..)
TA	Okay. And you, g1?
g1	I start with pentyl bromide .. I will slowly add that .. to the ethoxide. And I want to take that in excess.
TA	So?
g1	So I am sure that all my pentyl bromide has reacted away .. at least for 99% .. because .. ah .. the reason is that it is easier to purify.

Such deliberations before problems occurred did not happen at all in the non-Esters groups. So I conclude that the educational context of Esters did improve students' understanding of synthesis-planning.

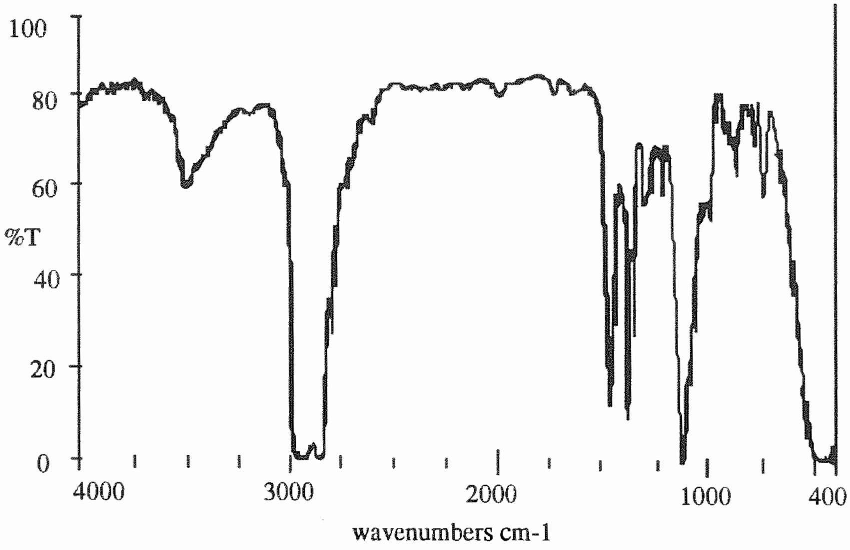


Figure 7.1 *Infrared spectrum of n-pentyl-ethyl-ether*

However, making rational choices based on synthesis-planning does not guarantee chemical success. Purification posed several difficult problems. In fact, only the students

starting with *n*-bromopentane and sodium ethoxide in ethanol managed to end with a reasonably pure ether. A representative infrared spectra is reproduced in figure 7.1. Clearly visible is the absorption at 1120 cm^{-1}, to be contributed to the ether. Also visible is an absorption at 3500 cm^{-1}, due to a trace of ethanol.
Those who started with the pentoxides in the corresponding pentanols were able to detect the ethers in their crude samples, but were unable to get rid of the pentanol solvent. The best attempt was made by a student who first filtrated off the NaBr precipitate, distilled off excess bromoethane, then added new sodium metal to convert the pentanol into the pentoxide, and finally wanted to distil the purified ether. Unfortunately, he discovered that the reaction between sodium and pentanol is very slow, so he couldn't complete his attempt within the time limits. However, this approach is very similar to the one proposed in Vogel's handbook on preparative organic chemistry on the synthesis of ethyl-hexyl-ether (Vogel, et al., 1989), p. 584).

In this respect I was not satisfied with Ethers 1. I thought I should try to give students a better chance at purification by not limiting the choice of a solvent to the corresponding alcohol. Although Ethers 1 corroborated several of my hypotheses, I thought it should be redesigned in this respect.

I was hardly able to investigate the second aspect of synthesis-planning: the application of new understanding acquired during this educational context. For this, it would have been necessary that students obtained an understanding of the side-reaction, preferably in terms of structure-activity-relations. However, students did not have enough time to complete their analyses, reflect on the results, and apply their interpretations again in synthesis-planning. Either the educational context had not been not appropriate, or I had been too ambitious to try to develop new understanding on all the themes in too little time.

7.6 Structure-activity-relations

In Ethers, an understanding of students' understanding of structure-activity-relations explains much of their actions concerning synthesis-planning and reaction-type. It is my intention that students will learn to use new theoretical structure-activity-relations for taking decisions regarding the reaction conditions.
In Esters, students had to learn to see a molecular structure in such a way that localized charges became an object of attention. I described their struggle to apply the appropriate issues of the Lewis formalism, such as electron pairs and nucleophility. From the point of view of the Lewis representation of structure-activity-relations, important features of the esterification mechanism such as the proton addition and the nucleophilic attack of the alcohol can be understood. The lecture course, taking place in the interval between Esters and Ethers, also deals with these topics. According to me, students should be able to pick up and apply the pieces of information and the associated vocabulary that deal with these localized charge effects. That is, they are able to recognize localized opposite charges in molecular representations and to recognize the consequent addition and substitution potential. The retrosynthetical approach elaborates on this issue. The obvious place to divide the ether molecule is next to oxygen. This leaves a fragment with a full negative charge on oxygen and a fragment with a full positive charge on carbon. They should be able to understand that the functional group that is attached to the fragment should leave

intact some of this localized charge. These opposite charge effects provide the rationale for a reaction between the substances: it will be a nucleophilic attack of oxygen on carbon. Although students may have a tacit understanding, McMurry mentions the issue explicitly. In this context, transfer of knowledge seems appropriate:

TA How would you make such a pentyl-ethyl-ether?
e7 That's in McMurry!
(laughter)
(...)
e4 Well ah .. it is easy if you .. for example .. you take an alcohol .. you put in a strong base .. I use Williamson .. you put in a strong base .. acid-base reaction .. then the sodium gets on the O .. and then, yes .. sodium and chlorine .. or ah .. sodium and that halide .. these run into each other .. and the rest runs into that oxygen and ah .. that's it.
(..)
e7 Yeah the reason .. if you have an alkoxide then you don't need to .. let it fall apart so to say .. then the H doesn't need to come off before it can react with that halide .. S_N2 substitution.

The topic of leaving group is dealt with during the lecture course, and students can make this into an issue:

g4 You have to have a good .. a good group that easily leaves.
(..)
TA What? Ah .. g4 .. please explain .. a good group that easily leaves?
g4 Some groups leave more easily in an S_N2.
g2 Yeah, bromine easily leaves.
g6 Bromine always is useful.

And:

h7 Chlorine is okay, bromine is better, iodine is better still, and tosylates.
TA Okay. How .. is that related .. is that a certain property that .. some are better than others?
h4 Acid rest of the strongest acid I think.
TA Acid rest of the strongest acid.
h3 And higher molar mass.
h2 Molar mass. The leaving group character.
h3 Yeah.
TA It has to be a good leaving group. It has to come off easily.
h3 Exactly.
h6 Electronegativity or something.

And:

TA Why should I take a chlorine, or a bromine, or an iodine, or a fluorine?
e1 Good leaving group.
e4 Tosylate, you can take that too, they are good leaving groups.
(..)
e3 Depends upon the electronegativity.
e5 Yeah.

The lecture course has informed students on what are good leaving groups, but it is important to note that the students do not really provide arguments that show an understanding of good leaving group properties. They certainly do not mention McMurry's argument, which is mentioned on page 342:

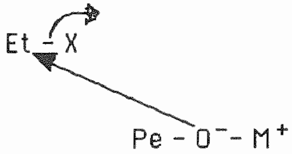
> Since the leaving group is expelled with a negative charge in most S_N2 reactions, we might expect the best leaving groups to be those that best stabilize the negative charge.

This is significant, since stabilization of charge is a form of delocalization, something the students, according to me, do not yet understand. Students instead seem to interpret the issue from the viewpoint of a force that attracts, instead of stabilizes, negative charge ("electronegativity or something"), notwithstanding the fact that the actual electronegativity value for an excellent leaving group like iodine is only 2.2, which is less than the value for carbon itself (2.5). Probably there is a relation between the intrinsic difficulty of delocalization and the fact that it is not clearly represented in molecular models. Mass is represented by the identity of atoms, space by relative position, localized charges by bonds and electron pairs, but to represent delocalized effects textbooks use vague terms like "stabilize" and concepts such as hyperconjugation and induction, which require intricate and laborious drawings. The issue of stabilization cannot be interpreted only from the viewpoint of electronegativity, as the students try to do.

In general, students follow McMurry's argument that ether can be prepared by an S_N2 reaction involving an alkyl halide and an alcohol or an alkoxide:

g1 You want to do an S_N2 reaction?
g4 Yes.
g2 Yes.
(...)
g2 Oh, according to me it can be done with an alcohol .. an alcohol and an alkyl halide.
(...)
TA Does everyone agree? Anybody other starting reagents?
g3 Well .. maybe the potassium salt of that CH_3 CH_2 4 times O.
g2 Yeah, also possible.
g4 Yeah, that's also possible.
g2 Or the sodium salt.

Drawings are made of the general process:



(..)
g2 The O is negative, that Br is delta minus, that C is delta plus .. it can't go wrong.

So far, so good. This is the expected basic scheme of the experiment. The students have adopted several important ideas from McMurry that are compatible with localized charge representation. Will they also pick up the caveat not to use 'more hindered substrates'? Initially, they do:

e3 But that salt .. is that with ethanol or with pentanol .. what is in that jar? In the book it says .. I think .. a sentence .. ah .. longer alcohols are better for the reaction or something. I don't know exactly what the sentence was, but .. it was in McMurry I think.
e1 Oh .. you mean .. more hindered alkoxide partners with less hindered .. halide partners .. is that what you mean?

And:

g2 The one that is most substituted gets the oxygen.
(..)
TA And that is wise? Is that what you want, or not?
g4 Yes, I thought so, yes. Ah .. yeah .. that's what you want, yes, because you want to ah .. to do that substitution .. the alcohol must be at the most substituted carbon atom.
(...)
g4 It is not so important for the .. attacking group .. say .. if it .. is sterically hindered by .. all those groups.
g1 It seems to me to a big hindrance.
g2 What matters is that the alkyl halide is less hindered than the alcohol group.
g4 Yes.
g1 But doesn't that decrease your yield too much?
g4 Well, yes, maybe it decreases.
R And why has it to be less hindered?
x2 Otherwise it goes .. that E2 reaction will then .. takes place too. And then you have two reactions. And you don't want that. That is why.
TA E2 reactions?
g1 Elimination reactions in which two particles are involved.
g6 Bimolecular so to say.
g1 Yes.
TA And what happens in that case?
g2 Ah .. what happens .. what is generated? I don't know by heart.
g1 Where's the book.
g5 An alkene, wasn't it?
g2 Yeah.
g1 Yes.
g4 An alkene, yes.
g5 A double bond.
g1 An alkene.
g2 Splitting off of an ah ..
g1 No, that's true .. an alkene is generated.
TA And why .. when does that happen?
g2 When your alkyl halide is more substituted.
TA That's when you get that alkene?
g2 Yes. Then you get that elimination reaction because that ah .. yeah .. ah .. well .. why .. actually .. did that happen?

There is no doubt that the students have read McMurry and are warned against the elimination reaction. This is a crucial moment in my experiment. One option, which would endanger my project of developing an understanding of the side-reaction, is that students would simply stick to McMurry and not engage in reactions involving a secondary or tertiary bromopentane. However, this is not what happened. The students' attention is drawn to elimination and this leads to a question concerning the reasons for this reaction to occur. The students appear to have no difficulty understanding the rationale of the alkoxide oxygen attacking the carbon atom of the alkyl halide in a nucleophilic substitution reaction. But they have difficulty imagining the elimination reaction:

h7 That Williamson synthesis .. S_N2 mechanism .. then ah .. with sterically hindered molecules .. won't go very good I think.
(..)
TA It is an S_N2 mechanism?
h7 Yeah, they say so.
h6 Ah .. oh yes it says so.
(..)
h7 And the O has to be at the least sterically hindered .. molecule.
TA O has to be at the least sterically hindered molecule.
h7 Yes.
h3 The most.
h4 Most.
h3 Most, I think.
h1 Umm .. he has to be at the most hindered I think .. otherwise you had troubles. E2 reaction could occur.
TA An E2 reaction.
(laughter)
TA Elimination.
h1 Yes.
R And how does that work?
(silence)

McMurry offers something that is a fact from a viewpoint the students do not yet have developed. In the context of the students, the only issue offered by McMurry they can make sense of is steric hindrance, and so try to find out why this is a disadvantage:

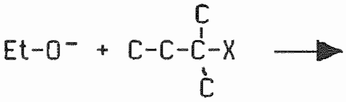
TA Here we have ah .. analogously .. this is tert-pentyl with an iodine and here .. the ethoxy .. a K .. is that not possible?
g2 No, because the nucleophilic attack .. that nucleophile .. with that O, you know.. it can enter nowhere for there is too much steric hindrance.
g5 Yes.
x2 Tertiary C atom .. and there is no .. ah .. no S_N2 reaction takes place. It doesn't fit in.
g4 Yeah.
TA So?
g2 So that reaction doesn't proceed, or very slowly.

There is no room for a nucleophilic attack. But does that explain the elimination?

TA Why don't you draw it?
h2 This one attacks the other:

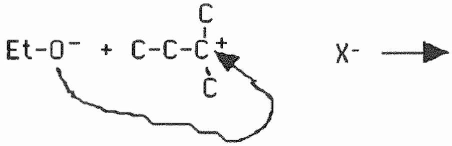
h6 Yeah .. that's what I thought .. and that on the other side that X goes away.
h5 Yes.
h2 The X goes away, yes.
h3 The X disappears.
h2 And if it is all right it would react with that H that still is there.

h4 Yeah, for the electrons of that O go to that R so it breaks an electron bond between the R and the X .. or is broken.
TA Okay. But I am not yet at that elimination you just mentioned.
h6 No.
h3 No, me too.
h6 No, but I don't understand why it eliminates .. or would eliminate.
h2 That's what McMurry says, but I don't know anymore.
h1 That's what McMurry says .. down below .. if it would be done reversed.
h2 Yeah, it was written below .. that is true .. but I don't know now.
TA If you would do it reversed you would get an elimination?
h1 But how it works I don't know.
h7 That was the elimination, like that.
TA Reversed, that is?
h1 The O at the least substituted.
TA So .. (..) the O has to be at the least substituted .. like this .. and with ethyl .. I'll write it down:



$$Et{-}O^- + C{-}C{-}\overset{\overset{\large C}{|}}{\underset{\underset{\large C}{|}}{C}}{-}X \longrightarrow$$

TA That's this one .. and here is an X. And that would somewhere ..
h1 That wouldn't give an ether.
h3 Elimination.
TA That wouldn't give an ether, according to you.
h1 Well, according to McMurry.
(laughter)
TA But you accept what McMurry says, so it is what you say. And .. this doesn't become an ether .. apparently. Why not?
h2 Well that O minus ..
h6 That has difficulty getting at that C or something.
h2 It cannot get at that C, yes.
h6 Yeah, I don't know.
TA Can't get at that C.
h2 Yeah, it all goes slowly you know .. I don't know, you know.
h6 Neither do I.
TA Well, have a go at it.
h7 Yeah .. ah .. where the O is .. it has to .. approach from the right .. at that X .. so it first has to .. the X has to come off [draws:]



$$Et{-}O^- + C{-}C{-}\overset{\overset{\large C}{|}}{\underset{\underset{\large C}{|}}{C}}{}^{+} \quad X^- \longrightarrow$$

h7 Something like this, yeah .. and that X has to come off first .. and then it can ..
h3 S_N1 .. that's what you get. It would be S_N1 in that case.
TA First this one off ..
h3 First this one off.
TA Do you notice that we are still not moving towards that elimination?
h5 No, I know that. I don't see it.
h6 No, but .. yeah.
h7 I don't know how that works.
TA Okay .. let us wait with that elimination .. first you get .. that X goes off.
h3 S_N1.

This conclusion was shared by other groups:

e1 Yeah .. when it has many substitution groups .. then it is S_N1, for that O has no room otherwise.

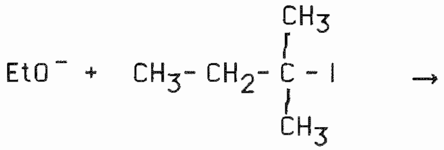
The students' efforts do not lead them to the elimination reaction, since they do not know how to see charge distributed in a molecular representation. In this respect, McMurry lets them down too. The book introduces elimination reactions on page 357 in a section called 'Elimination Reactions of Alkyl Halides' as follows:

> We began this chapter by saying that two kinds of reactions are possible when a nucleophile/Lewis base attacks an alkyl halide. Often, the reagent will attack at the carbon and substitute for the halide. Alternatively, though, attack at hydrogen can occur, resulting in elimination of HX to form an alkene.
>
> Elimination reactions are more complex than substitution reactions for several reasons. There is, for example, the problem of regiochemistry–what products result from dehydrohalogenation of unsymmetrical halides? In fact, elimination reactions almost always give *mixtures* of alkene products, and the best we can usually do is to predict which will be the major product.

And McMurry goes on discussing which products are formed. Not a word on what makes the attack on hydrogen as such intelligible.

The students' drawings do not even contain the hydrogen atoms, prone to elimination as these reportedly are. They see only one place for the oxygen to go to: the carbon atom. So instead, the students stumble upon the first order nucleophilic substitution. My interpretation of what happens is that the students use this mechanism as an escape clause. They are uneasy with the fact that they cannot grasp the elimination and yet cannot ignore it, since it comes from the most reliable of sources, the textbook. The S_N1 mechanism offers them the possibility of sticking to what McMurry says ('do not use hindered substrates') and combining this with a plausible explanation. This explanation is that S_N1 is slower than S_N2, and therefore it does not work. This is beautifully formulated in yet another group, in which a very similar discussion took place:

TA Which one of these two will have preference? [draws on the blackboard:]



$$EtO^- + CH_3-CH_2-C(CH_3)_2-I \rightarrow$$

$$PeO^- + Et\ I \rightarrow$$

f7 The second.
f3 The second, yes.
(..)
f3 It is simply .. that it can get there easier. That what it's all about, isn't it? And the upper .. well .. there you have that two methyl groups .. well .. they are in the way.
(..)

f6 The upper one will go very slowly. Because .. you say .. that I gets off spontaneously .. but that will not go like, hurray, here I go .. it will take some time I think. Will be slower .. the other one simply attacks .. and that simply happens through an S_N2 .. and when they meet then it's okay. But .. with the upper one .. has to .. that ethoxy must wait until that I is off before it can attack. So the upper one will most likely take much longer.

So now the problem has been redefined. Instead of focusing on elimination, whatever that may be, the students shift their attention to explaining differences in speed between S_N2 and S_N1. This issue proves to be not too difficult. A first explanation is given above: S_N1 is a two-step mechanism instead of a one-step, and this extra step will take extra time. This sounds plausibly enough. Another explanation is found in an interpretation of the stability of carbocations:

f6 I think the tertiary will go slowest of all. That one is the most stable. At least, that carbocation is the most stable.

The modifier 'stable' is apparently interpreted in an unintended way. The students remember McMurry's ordering of carbocations on page 180:

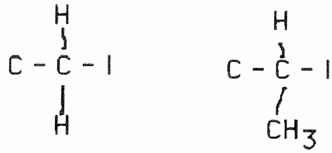
> Trisubstituted (tertiary, 3°) carbocations are more stable than disubstituted (secondary, 2°) ones, which are more stable than monosubstituted (primary, 1°) ones.

They apparently take this to mean that stability indicates inertia, lack of reactivity, whereas McMurry means the opposite. Another rationale is found in applying the viewpoint of steric hindrance to the attacking *tert*-pentoxide or pentanol:

g1 The yield is lower because of that steric hindrance of that OH.
g2 Well, then you should take the salt.
g4 Well I 'm not sure about that. Maybe. (..) What are your arguments for that?
g2 For what?
g4 Well .. that it does lead to loss of yield.
g1 Well .. because of that steric hindrance. Those CH_3 groups seem to me to be rather big, compared with that OH. So they will have an effect on the possibility to reach that Br group.
x5 Yes, but anywhere you cut it off, in both cases you will have steric hindrance.
g1 But it is slower.

The students tentatively conclude that *tert*-bromopentane can be used to make ethers, but they expect that it will be much slower. *Sec*-bromopentane would be less of a problem, just a little bit slower than *n*-bromopentane:

f7 Here you got one place less .. if you would write it down completely, with all the H's .. with secondary you got one place less .. where that O-atom can attack .. with the n-chain you have two places where that can happen.
TA How .. how do you mean that?
(..)
f7 Yeah .. ah ..
TA I'll draw it .. H .. H .. C .. and I:



f7 Yeah ..
f4 A methyl group is bigger.
f7 Because there are two H's .. and there is a CH_3 group .. a CH_3 group .. that will ah .. the ethanol ion .. will be more frightened by that methyl group I think .. and only go for that place.
TA So you say: this one is more sterically hindered? What consequences can that have?
f7 Amm .. the reactivi .. how quick the reaction will go.

No mentioning of elimination any more. Between *n*-bromopentane and bromoethane, the students do not see much difference:

TA Okay. Umm .. g5 .. you say you want to make the *n*-pentyl-ethyl-ether. Ah .. g1 said: it doesn't matter which two starting reagents you take, he takes the one potassium salt or the other .. that doesn't matter here, he thinks.
g1 No.
TA Does it matter to you?
g5 According to me it doesn't matter.
TA Doesn't matter? And g8? What do you think?
g8 Hmm .. I don't think with this one because you ah .. no steric hindrance .. and if you've got that, I mean steric hindrance, then it matters. But here only one of the carbon chains is longer. But .. it could be .. I am not really sure.
TA Yes? So it doesn't matter to you?
g8 Well, we could try it.

And that is what all groups do: they try every combination, expecting to find differences in reaction time, but no longer explicitly expecting elimination. This *piece de resistance* has been reasoned away. I conclude that, from the hermeneutic viewpoint, the students cannot take a viewpoint from which elimination becomes a meaningful issue, because they do not yet understand the corresponding structure-activity-relation. This implies that, to understand elimination, they have to experience the phenomena (the chemical activity) to develop a representation themselves. I hoped that the experiences with chromatography and infrared and the related discourse would be strong enough to achieve this.

Side-reactions like this elimination in general do not occur by chance. In this case, the side-reaction can be seen as an effect of enhanced reactivity. The nucleophilic disposition of an alcohol towards an alkyl halide is not very great. In other words, an alcohol is not a very strong nucleophile. Prolonged heating of mixtures of these alcohols and these alkyl halides does not lead to ethers. Williamson understood and remedied this. He increased the nucleophility of the alcohol's oxygen by replacing hydrogen with an alkali metal. However, by doing this, he also increased the Lewis base properties of the oxygen atom. This Lewis base is strong enough to attack weak Lewis acids, such as the bromopentane's β-hydrogens. Increased reactivity thus is accompanied by reduced selectivity. I have found no indication that students understand this duality. Some students call the alkoxide a base, but it seems to me that this is simply echoing McMurry. Hence, the initial group discussions do not lead to the expectancy of side-reactions because such a strong Lewis base is involved in certain mixtures. So it must be the experience of the side-reaction that has to reopen the discussion.

My intention was that students would reflect again on the basis of their actual experiences with the reaction. However, in Ethers 1, structured discussions concerning structure-activity-relations hardly occurred at the end of the experiment. Many students were still struggling with identifying the side-product the moment the experiment had to be ended. Thus, an application of new understanding to synthesis-planning was not achieved. I apparently did not prepare the educational context with enough rigour. So the development of the students' understanding could not be studied in enough detail, which implies that I have to return to this issue in the next cycle of Ethers.

7.7 Reaction-type

It will be clear from students' initial understanding of structure-activity-relations as outlined above that they did not anticipate the new reaction-type. But if they were to apply their actual understanding of reaction-type, they could develop attention for the side-reaction. The students have learned from Esters to meditate in advance on the mass balance from the points of view of reactions that come to completion, form a by-product, and/or form an equilibrium mixture. There was a marked difference between the groups that did not participate in Esters and the groups that did. The first groups hardly paid explicit attention to these issues, the second groups did. It was not really spectacular, just an increased and helpful awareness of the dangers that threaten a good chemical result:

h6 Maybe it is again an equilibrium reaction.
h5 Yeah, that's what I am afraid of too. Well, we'll see.
(..)
TA What kind of equilibrium do you think you could have? Between ether .. apparently .. and the starting reagents.
h6 Well .. I don't know .. how well does sodium bromide dissolve?
(..)
TA What does it mean if it's equilibrium?
h3 Less product.
h6 Yes.
h3 You'll find out when you analyze the samples. When the amounts do not change anymore you've reached an equilibrium.
h7 But when that NaBr precipitates ..
h4 That sodium bromide .. does that dissolve well in the solvent, or not?
TA In alcohol? In general .. not soluble, no.
h6 It does not dissolve very well? Yeah, in that case the reaction goes to completion.
h7 Yes.
h2 Yes.

This accurate conclusion influenced the students' synthesis-planning. They concluded that it is not necessary to use a large excess amount as they used in Esters.

More interesting is what happened concerning the side-reaction. I first mention a case of chemical success by serendipity that had to do with the use of silver oxide. My own experiments showed me that it was futile just to mix an alcohol and an alkyl bromide and add solid silver oxide. Some students did it this way and came up with no results. This was a disappointment for them, since the procedure had appeared so easy in McMurry.

However, one student had figured out that in the reaction of alcohol and bromoalkane, HBr could be generated. In the pre-lab discussion, the students had turned down the sulfuric acid method as inefficient because of the formation of symmetrical ethers. This reaction takes place in a strongly acidic environment. He therefore thought he should neutralize the HBr, and he did this by adding solid KOH to his refluxing mixture of ethanol, *n*-bromopentane, and solid silver oxide. To my surprise, but not to his, a reaction took place. The silver oxide appeared to go into solution and solid NaBr precipitated. Silver apparently was reduced, since the reaction flask eventually was coated internally with a silver metal mirror. The chromatograms revealed the generation of a product with exactly the same retention time as *n*-pentyl-ethyl ether. The presence of an ether was confirmed by IR. Especially interesting was the fact that his crude sample hardly contained pentene, and less than the corresponding samples of those starting with sodium ethoxide as the nucleophile. With hindsight, I can understand that KOH enhances the nucleophilic properties of ethanol without turning it into a strong base, whereas the silver probably forms a complex with the bromide, making this an even better leaving group. Essential seemed to be that silver oxide dissolves in this basic ethanolic medium, since it seems to act as a homogeneous catalyst instead of as a stoichiometric reagent, as suggested by McMurry. The same procedure, however, did not appear to work for pentanol.

From the point of view of reaction-type, it appears as if this student already applied an understanding of the side-reaction. However, the side-reaction caused by the sulfuric acid method had been discussed explicitly on the basis of a piece of textbook information. The group concluded that they did not want to use the sulfuric acid method because of the formation of three different products. The student's application of this conclusion was restricted to this same reaction. If he had understood the issue of side-reaction in a generalized sense, he would have applied it with respect to the elimination reaction, too. This, however, was not the case.

No student appeared to interpret experiences in terms of a side-reaction. Thus, the information provided by textbook and lecture course was not applicable. As reported, all groups of students decided to investigate several combinations of starting reagents, among them *n*-, *sec*-, and *tert*-bromopentane with sodium ethoxide in ethanol, and *n*-bromopentane with silver oxide and ethanol. I had tried these combinations before, so I knew what to expect chemically. I expected the first mixtures to yield two products, the ether and the pentene. With *n*-bromopentane, ether would be the dominant product, with *sec*-bromopentane the alkene would dominate, and with *tert*-bromopentane there would hardly be any ether detectable. With silver oxide, I expected that nothing would happen.

The students put together their reagents in a reflux apparatus, and within minutes a white-yellowish precipitate appeared in all the alkoxide combinations. The students took this as a sign of the desired reaction taking place, took samples, and made gas chromatograms. They continued refluxing until the chromatograms stopped changing. After that, second group discussions took place to discuss the results. In all groups a similar thing happened. Several students reported unexpected peaks in their chromatograms:

TA	Were you able to identify all your peaks?
e1	No, not everything.
e7	No, I've got too many.
TA	Do you .. do you have strange peaks?

e6 Yes.
e7 Yes.
e1 Yes.
(..)
TA Yesterday .. we were discussing .. maybe different things can happen .. or maybe people see something different in their chromatograms .. I told you to think about that .. whether something different actually can happen, or not. What do you think?
e5 Other reactions or something?
e4 Yeah with that ethanol that is ..
e7 Yes, with me that ethanol also became an ester.
R Ether.
e7 Ether yeah. For I also have amm .. what's its name .. pentoxi .. sodium pentoxi .. and when you do that with that etha .. ethanol let it react .. than you also get that ether. So that is just two ways to go to the same substance.
TA So in principle there is no other product if that would happen.
e7 No. But I do have too many peaks.

And:

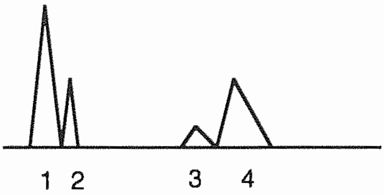
h3 Well .. I have .. just after ethanol .. there is a small little peak. I don't know what that is.

And:

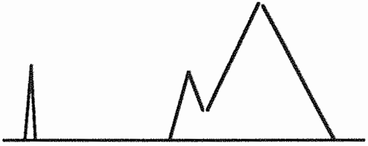
TA Is ah .. do you think it is over .. that it is .. everything has reacted? The starting reagents?
g5 Yeah .. well .. I don't know .. with that sodium ethoxide I don't really know. Cause I have yet another unclear peak in my chromatogram. Of which I don't know what it is.
g6 But .. it can't be ethoxide .. it doesn't detect that.
g1 No.
(..)
g5 But yeah .. I would say .. when that .. when the bromopentane is gone .. then the sodium ethoxide should be gone too, if it reacts one to one.
(silence)
(..)
g5 Yeah. It is this one peak, of which I don't know what it is. Oh, and it is not sodium ethoxide, so I have something extra in it.
TA Plus something extra.
g5 Yeah, I don't know what it is.

In the same group, one student (g6) had started with *sec*-bromopentane, another (g2) with sodium *sec*-pentoxide:

TA G6, what did you do?
g6 I have *sec*-bromopentane .. and I have that sodium ..
(..)
g6 But my chromatogram simply is a mess.
TA And what .. what do you have? (..) Could it be that side-products have been formed?
g6 No.
TA No. How does it look like?
[g6 draws a chromatogram on the blackboard]



TA Ah .. but how many products?
g6 Ah .. this is the last.
TA One two three four substances.
R And what is what?
g6 One is my ethanol .. that second one it the big unknown .. the third is probably .. or that .. is bromopentane and in that case the fourth I hope is my ether.
TA And if you compare that with g2 his spectrum?
g2 What do you want?
g6 The last.
g2 The last .. that is this one [shows a chromatogram that looks like this:]



g2 This ..[points at the second peak] is my ether. I am dead sure about that.
TA And you have .. you have pentanol, do you [points at the last peak]?
g2 Yes.
g6 If that is your ether, that is my ether too.
(..)
TA And you have a something that is a question mark?
g6 Yes.
(..)
TA And you don't have a question mark substance?
g2 No.
TA And g6 has.
g6 Yeah. Funny, isn't it.
g2 You see, when I do something, it works.
(laughter)
TA Maybe it is the route.
g2 Yeah, maybe.
TA Or maybe it is g6.
g2 Maybe.
g6 I think so.
(silence)

Similar discussions also occurred during the lab sessions themselves. The students noticed the extra peak and expressed their surprise and unhappiness, but nobody related this peak with the elimination reaction discussed previously. This indicates that textbook information that is not understood cannot be applied in practice, not with respect to the straightforward goal of making the product, and certainly not for investigating the process from a theoretical viewpoint.

In the educational context of Ethers it is crucial to draw students' attention to the issue of the identity of their second product, since they apparently cannot deduce this identity from their textbook knowledge. At this moment students predominantly focus on making the product. They hope that the unknown is an artefact that will eventually disappear. They therefore did not push the quest for the identity but instead started with purification. In this respect, it appears that the educational context is too dependent upon the TA. It would be his or her job not only to guide students to the product, but also to support them to pursue more theoretical questions within the format of simulation-of-research.

I also appeared to have been too ambitious. Within the given time, only a minority of the students was able to complete the purification and identification stages with satisfactory results, that is, with answers to their own questions. I noticed that identification was initiated late. Students first wanted to purify their products completely before attempting to identify them with infrared. This analysis could be initiated somewhat earlier. Another problem was that the students, not knowing the identity and physical properties of the second product (the pentene), were not very successful in isolating. One student distilled the crude mixture, expecting to collect *tert*-pentyl-ethyl-ether at about 100°C. So he collected a fraction around this temperature and threw away what came before, which, according to him, was only ethanol. GC analysis identified the product as a mixture of ethanol and *tert*-bromopentane, whereas the product peak, that had appeared in the crude synthesis mixtures shortly after ethanol, had disappeared. He had noticed, though, that the first distillate fraction smelled awful. It appears that students were unable to shift towards another goal during the process. I had expected that they would shift their attention towards isolating and identifying the unknown product. Instead, they rather ignored this product, or maintained that it was the ether. They choose their purification and identification activities accordingly. I conclude that, although students do have experiences with the side-reaction, the educational context fails to cause reflection and experimenting from the viewpoint of the structure-activity-relations.

In the final groups discussions, the general conclusion can be represented by the following fragment:

TA There are a lot of strange GC peaks around ethanol .. and nobody says .. I know what it is. (silence)

Only one group revisited the elimination reaction:

h7 With me .. well .. not much happened .. well .. I think I have made ethanol.
TA Ethanol?
h7 Yes.
TA How's that? From sec?
h7 Yes.
TA And no product?
h7 Not an ether, no. There is a little peak after ethanol, but I don't know what it is.
TA And tert?
h8 Nothing.
TA Nothing.
h8 A reaction did occur .. I looked it up in McMurry .. we had almost identical substances .. same mechanism .. and that resulted in a pentene.
TA Pentene? And you also found that in your gas chromatograms?
h8 I don't have .. found nothing. Maybe it is that peak .. at the same place as ethanol ..
TA You say: I have made a pentene, or ..?

h8 No, I don't know, but there was a reaction and I wasn't able to find ether in the IR. Must have been another substance being formed.
TA A reaction .. no ether .. and you say, pentene? And then?
h8 Purification was not a success.
(..)
h7 We lost it .. the product.
(..)
h3 With that tertiary .. that one .. that should be according to .. it was an .. an S_N1 .. that should be possible in principle .. that the bromide .. leaves the .. pentane .. but that apparently doesn't happen.
TA That bromine would dissociate from the pentane and then the ethoxide would attack?
h3 Yeah, yeah. That's what I mean.
TA Those two steps after each other. If it would go, it would go like that, but ..
h3 But, well, that doesn't happen.
TA That doesn't happen.
h3 Maybe something with the theory.
TA Ah .. as far as I know .. what is in the theory .. with that tertiary .. what was written exactly?
h2 E2 elimination .. takes place.
h7 E1 .. wasn't it?

The group discussions in this group and in the other groups end with the TA and me giving an interpretation of all the phenomena and an explanation of the side-reaction and the mechanism. A student reacted:

h6 Well, according to me some of us said that during the first discussion .. wrote it on the blackboard .. I don't remember who it was .. that there really could be side-reactions .. but when they happened to be there .. we just didn't see it.

7.8 Simulation-of-research

Unlike Esters, the educational context of Ethers is not dependent upon tasks. An introductory question (how to make unsymmetrical ethers) and a suggestion from literature (the Williamson method) put things in motion. The students worked as a group, distributed and compared different approaches, and put the stress on what they thought was important. The advantage of this format is that students really can pursue their own questions, determine their own methods, and set the criteria for the results. I discovered that the format also has disadvantages. In the first place, the role of the TA has become more difficult. Although I provided the TA's with a manual in which my ideas, my objectives, and the outcomes of my own experiments were described, they had much difficulty in applying this information. It was not derived from their own understanding. In the second place, the format allows for very divergent student ideas. It was sometimes difficult to judge whether the ideas were feasible, especially for the TA's, who often lacked sufficient understanding of laboratory procedures and did not have much experience with doing chemical research and pursuing theoretical questions themselves.
A conceivable consequence was that both the students and the TA settled for obtaining the ethers. From a research point of view, trying to adopt an already existing approach to a few specific compounds is a rather humble goal. Although the students had to go through the procedure, make adjustments, interpret ambiguous results, and theoretically explain unexpected deviations, their activities were meaningful mainly from the viewpoints yield and purity.

Most of what the students were doing can be seen as application of theory in the context of making products, not as verification or investigation in a theoretical context. As I described, some students initially were reluctant to start with *tert*-bromopentane, since this substance is sterically too much hindered to participate in a second order nucleophilic substitution. However, other students pointed out that it could also react through a first order nucleophilic substitution, by first dissociating into a bromine anion and a carbocation. This reaction, as students thought, would only take more time, but would also lead to the desired ethers. So they conducted the reaction, probably initially with the idea to compare S_N1 with S_N2. But they lost this viewpoint when they became engaged in the synthesis itself, focusing on making the ether instead. Thus, the format of simulation-of-research did hardly succeed in advancing theoretical questions concerning the structure-activity-relations.

Although the focus was on making ethers, it was clear that the students expected to be judged on the basis of the quality of their participation in discussions and actions, and not on personal yield and purity. Some students, especially those who embarked on the silver oxide approach, never reached any positive chemical result. Still, this was seen as an unavoidable possibility within this context, and not as a failure. Although students understandably paid most attention to their own attempts, they understood that their attempt was part of a group effort. Now and again, they abandoned their own fruitless attempts to help others whose endeavours seemed more promising.

7.9 Ethers 2: changes in the educational context

Since I did not achieve all my goals with this first version of Ethers, I decided to redesign the educational context. First, I gave more detailed advise to the TA's. During the teacher training I put more stress on the format of simulation-of-research. I emphasized that the goal was not just to make ethers, but to pursue questions and hypotheses, especially with regard to theoretical structure-activity-relations. The TA would have to stimulate these questions, organize discussions on preliminary results, and give opportunity to apply new understanding of structure-activity-relations to synthesis-planning.

I also advised the TA's to pay early attention to identification. When chromatographic analysis would reveal the generation of a new substance, the TA should advise students to identify this substance. In my opinion, infrared spectroscopy is the most suitable technique to employ in this situation. M&M1 does not have its own NMR or GC-MS equipment, nor are the students able to interpret NMR or MS spectra. Although it would be possible to send samples to a service department and have them analyzed and interpreted, this would take too much time, and it would not be students' own interpretation. On the other hand, M&M1 has its own IR equipment, and I anticipated that students would be able to grasp the central idea of this technique, that is, functional groups can be recognized by the infrared absorptions at specific places in the spectrum. To understand this, students just have to understand the representation of substances by molecular formulae featuring atoms and bonds. In fact, the infrared spectrum of a substance is a structure-activity-relation. In this context, the activity is not chemical but physical in nature: the substance reacts to an electromagnetic field in a way that depends upon its structure. With the help of a table, the students can analyze IR spectra of their samples regarding the presence of functional groups. The presence of ethers would be revealed by the presence of an absorption at about 1120 cm^{-1}. In order to help students, I prepared spectra of pentanol, bromopentane, bromoethane, and diethyl ether in advance. Since alkenes also have rather specific IR absorptions, I thought it would be possible that students would identify alkenes in their samples, when these are present.

Second, I made the sodium pentoxides available in a wider variety. In Ethers 1, these reagents were available only in a solution of the original pentanol from which they were made. In this way, I created a very difficult separation problem for the students, because it is difficult and time-consuming to separate the pentyl-ethyl-ethers from the pentanols. The pentanol solutions were still available, but I also prepared alcohol-free sodium pentoxides by heating and stirring powdered sodium and a stoichiometric amount of the pentanols in ortho-xylene under nitrogen at 90°C. After the sodium had disappeared, the solvent was removed by distillation and the last traces drawn off under diminished pressure (Fisher & McElvain, 1934). In this way, sodium *n*-pentoxide and sodium *sec*-pentoxide were prepared and kept under nitrogen until use. It appeared that sodium *tert*-pentoxide is soluble in ortho-xylene (Conia, 1950; Fieser & Fieser, 1967), so I prepared this reagent as an ortho-xylene solution. My intention with these wider variety of reagents was to draw attention to the role of the solvent in the synthesis of ethers.
The solid pentoxides also dissolve in dimethyl sulfoxide (DMSO) and other polar aprotic solvents and can be made to react with bromoethane in the Williamson method. I therefore prepared these solids, in case students would want to use such solvents. However, the pentoxides are highly sensitive to water vapor from air, so it is unavoidable that some pentanol would result when the relatively inexperienced students would handle these reagents. In fact, this behavior of the pentoxides is an example of high reactivity combined with low selectivity, leading to various side-reactions. Since students do not yet understand the side-reaction, I cannot expect that they will anticipate this issue. I therefore decided to ignore this little drawback. When students have mastered the new reaction-type, the problems of reactivity and selectivity could be the theme of a subsequent extension of the educational context.
The pentoxides only dissolve with some effort, but the subsequent reaction with bromoethane is strongly exothermic. Also, isolation of the ether is not completely straightforward. Extraction with first adding a highly apolar solvent such as diethyl ether or pentane followed by adding water seemed to work best. In this way it is possible to separate the ether from DMSO.
I took advantage of the fact that sodium *tert*-pentoxide dissolves in ortho-xylene. In Ethers 1 it became clear that both steric hindrance and certain differences between S_N2 and S_N1 are understood by the students. They know, for instance, that polar media favor dissociation and therefore enhance the possibility of S_N1. In this case, something analogous is the case. In ortho-xylene the sodium *tert*-pentoxide does not dissociate. Since the reagent also is sterically hindered, this negatively influences its reactivity with bromoethane. The reactivity can be enhanced appreciably by adding DMSO to the medium, since this favors dissociation of the sodium *tert*-pentoxide. I was interested whether students would investigate this line of thought, since I anticipated that it would be within their reach. This theoretical question could follow from students' experiences with this reaction.

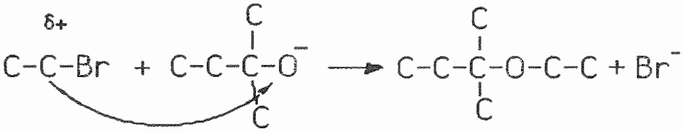
Ethers 2 was carried out by two groups of students that previously had carried out Esters 4. Several things went as I had anticipated. The students conducted comparable discussions as in Ethers 1 and made similar choices. That is, they discussed McMurry's statement that the use of the more hindered alkyl halides leads to elimination, but they nevertheless carried out these reactions. A difference was that there were now more ways to carry out the reactions. Some students used solutions of the pentoxide in DMSO, and although not all of them succeeded, some achieved satisfying chemical results. The early use of infrared for identification proved successful too. Some students identified the alkenes and were able to combine this experience with McMurry's information. Experiences with the xylene solution led to an important discussion on steric hindrance and reactivity.

7.10 Reaction-type, structure-activity-relations, and synthesis-planning in relation

In interpreting Ethers 2, I focused especially on the mutual relations between the issues. As I pointed out, decisions with regard to reaction conditions are based on the existing understanding of structure-activity-relations and reaction-type. So, initially, the students will not anticipate the side-reaction since they do not understand the relevant structure-activity-relation. If their actions generate experiences that draw attention to the side-reaction, and if they also foster a theoretical interest, then they can develop new understanding of structure-activity-relations. This in turn can then be applied to synthesis-planning.

Initially, similar events took place with respect to the structure-activity-relations relevant for understanding the elimination mechanism. Students discussed the Williamson ether reaction in terms of localized charges:

i4 I would take .. an alkyl halide and an ah .. an alcohol with sodium .. or potassium .. I don't know how that is called.
TA An alkoxide.
i4 Well .. take for example bromoethane .. I don't know if that is available .. but .. you just let it react with that ah .. alkoxide and then you get an S_N2 reaction. [draws on the blackboard:



TA Is that clear? Does everybody understand that?
i4 This carbon is somewhat positive .. because of that bromine. That one attracts electrons .. that's why it is positive .. and the other one has electrons too much .. so this one attacks at this place .. because it is negative .. and then this bromine splits off.
i8 It can also be .. instead of that bromine .. can be an iodine or a chlorine.
TA Ah .. why?
i8 Hmm .. yeah .. because that groups also are negative .. they can split off too in an S_N2 reaction.
TA And this is an S_N2 reaction?
i8 Yes. That's what we just learned.

Some students introduced into the discussion the facts regarding the use of hindered alkyl halides mentioned by McMurry:

TA Is it pure accident that you made a drawing with the ethane halide and the *tert*-pentoxide?
i4 Ah .. what do you mean?
TA Well .. ah .. could you do it just as well with .. say .. bromopentane and ethoxide?
i4 Well ah .. this one .. the alkyl halide .. has to be ah .. secondary or primary .. and not tertiary .. because that is sterically hindered.
TA It has to be primary or secondary?
i4 Yeah. Secondary is still okay, but tertiary won't work.
TA Why not?
i4 Because it is hindered sterically. The oxygen can't get there. Can't attack.
i5 Yeah .. you get .. alkenes do you get.
i6 You get E.
i4 Yes.
i6 Yeah .. you get .. e .. li ..
i8 An E-reaction.
TA A what?
(laughter)
i4 Elimination.
i3 Can't you get an S_N1 in that case?

The discussion went on but the students did not succeed in representing the elimination reaction. Again, the S_N1 mechanism seemed plausible to the students:

i5 Well .. that S_N1 .. I think that is possible. Yeah .. that it first .. gives up a Br minus .. and then ..
i4 But .. this one ..
i5 Hmm .. well .. okay .. but you can just as well ..
i4 Yeah .. this one is plus .. in that case .. so the other could attack it .. probably.
(..)
i1 But it will be much slower .. secondary and tertiary will go much slower.

The discussion then moved to other topics. Eventually, the students wanted to try a wide variety of combinations of reagents, among them the sterically hindered bromopentanes with sodium ethoxide. However, a clear interest in theoretical questions did not emerge. Students focused in their discussions on how to make the ethers. Structure-activity-relations were used to determine whether certain routes were feasible or not. The reverse–using a reaction pathway to determine certain structure-activity-relations–did not occur spontaneously. Nor was the TA able to induce these questions.

As a result, student i4, who had initially objected to certain pathways because of steric hindrance and elimination, could now be found in the laboratory trying to make *sec*-pentyl-ethyl ether from *sec*-bromopentane and sodium ethoxide. I decided to follow closely what would happen. I tape-recorded the discourse that took place during the lab work. We both concluded from the precipitation of a white salt that a reaction took place. I4 made several gas chromatograms during this process, and concluded that the amount of sec-bromopentane was diminishing whereas at two places new peaks came into being:

R Well .. how are you doing?
i4 Very well .. I think. At least .. it reacts .. there is a lot of that NaBr at the bottom. And there are new peaks.
R Great. What does it look like?
i4 Here .. [shows chromatogram] .. this is ethanol .. that is the solvent .. and this is the *sec*-bromo. This one is at the beginning .. before it started refluxing. And this one [shows another

chromatogram] is later and this one [shows third chromatogram] is how it is now. And there are these new peaks. I think that must be the ether.
R Yeah? Both peaks?
i4 Well .. I don't know. I thought .. with chromatography .. every substance has a peak, hasn't it?
R Yes, that is the idea. Sometimes .. it won't get through .. you know ..
i4 Yeah .. like we had with that esters .. there was something .. a substance .. that you just couldn't see with it.
R Yes. But here you have two new peaks?
i4 Yeah. Well .. yes. Maybe .. something .. or not.
R What do you think it can be?
i4 Ether. I don't know. Maybe .. impurities or something?

At this moment there was no reference at all to the elimination reaction or to the formation of alkenes in the case of secondary alkyl halides. Later, attempts at identification took place with infrared spectroscopy. The students used a chapter in Vogel (Vogel, et al., 1989), pp. 273-316) to interpret their spectra. I4's spectrum is represented in figure 7.2.
The TA had provided the students with a spectrum of diethyl ether, and had told the students to look for similarities and differences. In comparison with the IR spectrum of this ether, i4's spectrum showed several differences. The large absorption at about 3400 cm^{-1} was easily identified by i4 as belonging to the O-H stretching vibration of ethanol. The C-O stretching vibration of ethanol can be seen at 1060 cm^{-1}. There also is some absorption at the place where the ether is to be expected, but it is a just little off the right spot. It should be at 1120, whereas it is at 1080 cm^{-1}.

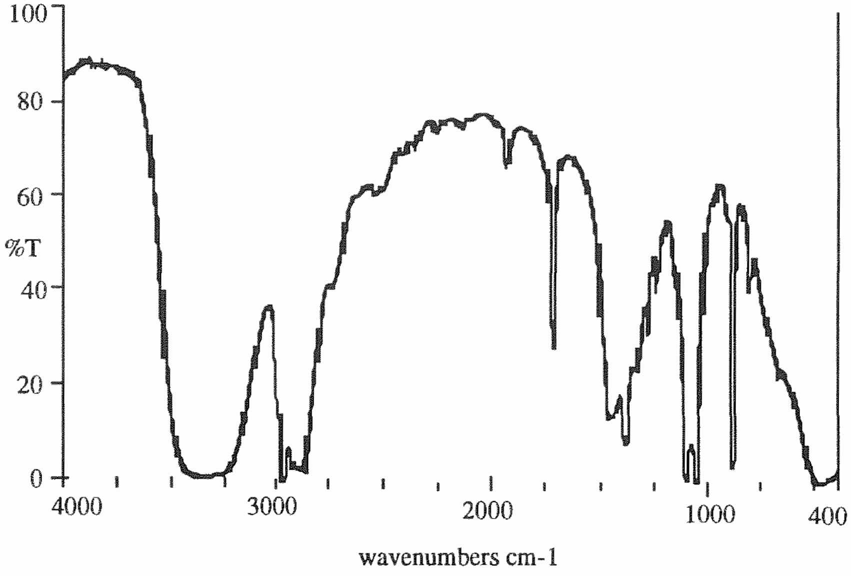


Figure 7.2 *Infrared spectrum of a crude product containing alkenes*

It took more effort to identify the absorptions at 860 and 1660 cm^{-1}. These belong to the =C-H bending vibration and the C=C stretching vibration, respectively.

R Well .. do you know what you've got?

i4 Well .. it looks like it. It is .. very complicated .. to find it all with this book ..

R What have you found until now?

i4 I think I've made the ether .. it is here .. [points at 1100]. But there also is ethanol .. I knew that from the gas chroma ..to .. thing. You can see it here too .. here this large thing .. it says that it belongs to the .. O-H stretching vibration. And this [points at 2900] is the same as in that diethyl. This .. [points at the 1250-1500 region] also resembles .. is the same .. but .. well not exactly .. but it is a different substance. But .. here [points at 1700 region] is something I don't know.

R What could it be?

i4 Well .. I am just reading the book .. to see if I can find it. It could be .. a carboxyl .. or an .. ah .. amide .. or .. amides, yes .. or alkenes. Alkenes also have something between 1000 and 800 .. I have something there too.

R Well .. do you think amides are very probable?

i4 No, not really. There is no nitrogen. And carbonyl .. that is C double bond O .. they are not there too .. I think. It also is not the right spot .. mine is at 1660 .. C double bond O is at 1720. Or doesn't that matter? But ..that leaves alkenes .. were would they come from?

(silence)

i4 Wait .. ah .. there was something .. McMurry said it .. what was it .. alkenes were formed when you used .. the .. more hindered .. alkyl .. things.

R Really?

i4 Yeah .. and that is .. I used the sec .. that is .. it could be .. maybe it is .. elimination takes place?

R Well .. what do you think yourself?

i4 Yeah .. well .. maybe these are .. alkenes .. pentenes. But then I have two of them .. there's one at 860 and one at 1660.

R Well .. yeah .. that is not really true .. I think .. they belong to the same substance .. could belong to the same .. it is just two different vibrations .. absorptions ..of the same bond .. at different places .. you know .. this is not chromatography.

i4 Oh yeah.

I4's confusion of an infrared spectrum with a chromatogram stood not alone. I had noticed several instances of students confusing the meaning of peaks in these pictures. In chromatography, every peak represents a substance and every substance can produce only one peak. In infrared, this is not the case: every substance produces many peaks, whereas specific peaks also can stem from different substances. For instance, since almost all organic substances contain C-H bonds, they will all have absorptions at 3000 cm^{-1}. However, I think this confusion is superficial and does not originate in a fundamental problem with understanding. I4's response to my explanation ("Oh yeah") seems to confirm this.

The issue was later discussed in group discussions too:

TA Shall we move on to the next one? We tried to make secondary ethers .. this one .. ethanol and sodium .. and bromopentane .. because we thought ..

i4 Ah .. well .. that one has failed .. some two alkenes are generated, so ah ..

TA Alkenes are generated?

i4 That's what I think.

TA Well .. can you explain how these alkenes are generated?

i4 By an ah .. E2 ah .. yeah .. elimination. Because a strong base is used .. ethoxide.

TA Hmhm.

i4 By that reaction of ethanol and sodium .. the ethoxide has taken an H plus from that bromopentane .. of a adjacent C atom .. and that made it more stable to form an alkene .. instead of going into that S_N2 reaction. And then .. he has formed two alkenes .. 2-pentene and 1-

pentene I think. And when you look at the chromatogram .. there you have .. the two main products are there .. ethanol .. a whole excess.

TA The starting reagents, yeah.

i4 And there is something at the foot .. against .. bromopentane .. that is ah .. still there.

TA *Sec*-bromopentane?

i4 Pardon?

TA The sec .. secondary bromopentane.

i4 Yes. Secondary. And when you look at the second .. yeah .. here at that first you already can see the two small peaks of the alkenes I think .. and when you look at the second you can see that the secondary .. bromopentane .. disappeared .. then there are two peaks that have grown bigger .. enormously bigger even.

TA Yes.

i4 And .. I think that must be the alkenes, because if it were an ether it should have been later .. I have heard that.

TA But how do you know that they are alkenes?

i4 IR.

TA IR. And how long did you reflux .. because you said .. the bromopentane is gone .. and that it had all become pentene. And did you also have some product?

i4 Yes, I think a little bit. Just a little bit.

TA A little bit.

i4 Ah .. I have .. I think .. wait .. refluxed .. for about an hour.

TA An hour.

i4 But .. according to me I don't have any starting reagent. Is gone.

TA No, so it makes no sense to go on refluxing.

(..)

TA And i2 .. you did almost the same as i4 .. did you also saw the formation of pentenes? I mean .. she has secondary, and you have primary.

i2 Well .. I have .. in the beginning .. I also have small things .. at the same place as she. But they are so tiny .. I mean .. almost nothing. Compared with the ether.

(..)

i4 I think you have them too. Yeah .. I think they are pentenes .. because .. the ratio you know .. in one case more pentene is formed than in the other .. and that is what is predicted by the reaction.

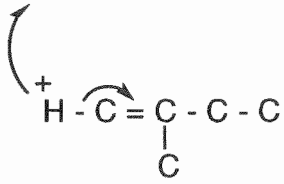
TA It is predicted that i2 hardly has pentenes, and with you, they are there?

i4 Yeah, I think so. I thought ..ah .. that the ah .. equilibrium .. is different. With me it is secondary, so there is much more hinder. So .. according to McMurry .. it is correct.

(..)

TA And how does it work?

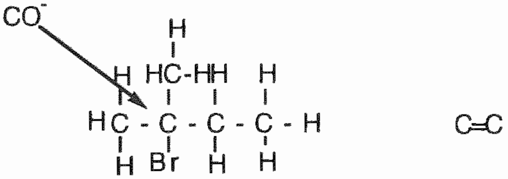
i4 Well .. when the Br is gone .. and the oxygen can't get there .. then an H-plus leaves .. like this [draws on the blackboard]



i4 And then you get this one .. you get an alkene. Because it is in solution .. and then .. so .. the Br is gone .. and it can't attack .. and then simply an H-plus leaves. Is more stable.

At this moment the discussion unfortunately took a different course, and the issue was not revisited again. So I am not really sure what it is that i4 meant with the word 'stable'. It seems clear that the textbook information at first had little influence on students' actions and interpretations. The experience of unexpected peaks in chromatograms and infrared spectra led to attention to the side-product. This product was identified and this apparently brought back into memory the textbook information. However, the students' rationalizations still lack delocalized quality. The rationale for elimination is given from the viewpoint of steric hindrance. But this is not a positive argument for elimination, it just makes substitution less likely and thus slower. Statements like "and then simply an H-plus leaves" are not bolstered by arguments. They are confirmed by experience and by the textbook, but they are not understood. Although Ethers had drawn attention to the issue, it has not completely succeeded in developing an understanding. Probably a more focused issuing discourse, in which the results with the three bromopentanes would have been compared and the students would have been asked to explicate their ideas regarding 'stable', 'strong base', and the like, would have helped. As it is, an incidental student recapitulated the textbook information, whereas most of the other students watched in silence. In the other group, a similar discussion occurred:

j1 We did .. we have tert .. in any case .. we have tert pentane .. and ah ..
j5 Bromopentane.
j1 Yeah ah .. Et O Na .. plus pentanol bromide .. pentane bromide .. yeah .. and that should have formed an ether ..
j5 Yeah but it didn't. There was that elimination.
TA Elimination?
j5 Yeah .. pentenes .. we had .. double bonds .. at 900 and at 1650 .. I think .. it was.
TA That was in the infrared?
j1 Yes.
(..)
TA But you said something about elimination?
j5 Yeah. [draws on blackboard]



j5 It takes off the H .. that becomes OH .. and then the bromine goes off too .. and then it is a double bond. That is because of that steric hindrance. It is an S_N2 reaction, but he cannot get in between, so this one goes off more easily than this one gets on it.
TA What is sterically hindered?
(..)
j2 Did you think this up yourself?
j5 It is in your organic book .. you should be careful .. that the O group is not attached to the wrong one.
j2 I don't understand a thing of it.

And again, the discussion drifts off to other topics without an explication or a convincing rationale for the elimination reaction.

Consequently, students did not reapply their new understanding of structure-activity-relations to synthesis-planning. The issue of synthesis-planning as such, however, was expanded to include the choice of a reaction medium. This choice is also related to structure-activity-relations, although not specifically combined with the side-reaction.

In Ethers 1, it was not possible to develop a viewpoint on this issue, because the choice had already been made. The pentoxides were available only as solutions in pentanol. In Ethers 2, the students could make their own choices. I anticipated that the students would prefer to perform the reaction in a homogeneous medium:

TA Do you need a solvent or something?
i4 Yes, that improves the reaction.
TA Why is that?
i6 Because it ah .. better mixes .. it is all mixed through each other.
TA Could it react as powder?
i5 Well .. not so fast.
i6 Yeah .. is it .. fine? Is it a powder? Does that matter?
TA Maybe when you grind it?
i3 I think it will react, but ..
(..)
i6 Let's just try it.

The students' apparently think that the chief function of a solvent is to secure thorough mixing of the reactants. So to check this, this group set up an attempt in which powdered sodium *n*-pentoxide was used in combination with bromoethane. It turned out that this was not a success, since no reaction took place.
Since sodium ethoxide is made from the reaction of sodium with ethanol, this last solvent is an obvious choice. It was used in all cases in which sodium ethoxide was used. However, students were reluctant to use ethanol in the case of the pentoxides:

TA What solvent would you use?
j6 Not water.
TA No? It doesn't dissolve in water?
j6 No, according to me you get .. it becomes the alcohol .. it will react with water.
j3 It is a strong base.
TA Okay. So apparently not water.
j3 Something polar.
TA Something polar
j5 A polar solvent.
j6 Ethanol again.
(silence)
j3 Maybe that could react too.
j4 Could exchange.
TA Exchange?
j4 Well .. that H of ethanol could go to that Pe O.

This reveals that they understand that a solvent should not react with the reagents. Sodium pentoxide does indeed react with ethanol in the way suggested. The choice of the reaction conditions thus is made from this point of view. Following this line, pentanol was suggested, but rejected, because they thought it would not be polar enough to solve the sodium salts:

j4 You need something polar that doesn't react. You have to take an .. aprotic polar solvent.
TA And what is that? Can you give an example?
j4 Ah ..
j1 DMSO.
j4 DMSO .. HMPA .. and there was another one .. acetonitrile.

The knowledge of these compounds obviously is an effect of the lecture course. As a result, several students started using DMSO. Chemically, handling this substance in combination with sodium pentoxide demands some experience. Both substances are hygroscopic and pentoxide is sensitive to air, which would imply that the reaction should take place under nitrogen. However, the students lacked sufficient experience and did not expect problems in this respect. They carried out their activities under atmospheric conditions. This resulted in some pentanol formation. Also, DMSO might decompose at elevated temperatures. The students were warned against this, and as a result they controlled the temperature of the DMSO solutions to keep it below 80°C. Sodium pentoxide does not dissolve rapidly in DMSO, and it took the students much more time than they had expected to produce a homogeneous solution. In two cases, bromoethane was added directly to the already warm solution. This resulted in a vigorous exothermic reaction, presumably between bromoethane and pentoxide, but also a foam was produced, probably because of decomposition of DMSO. Since it took much effort to dissolve the pentoxide, the fact of its subsequent vigorous reaction need not have been a surprise. Apparently, the pentoxides are brought in an energetically unfavorable condition. This experience could have been a suitable issue for discussion. However, the students did not reflect further on these phenomena; they were too occupied with the practical problems. Eventually, a clear reddish solution remained. GC analysis revealed the presence of a new product and of pentanol. Direct infrared analysis of the crude product was not possible since DMSO would attack the infrared cells, which are made of DMSO soluble sodium chloride.

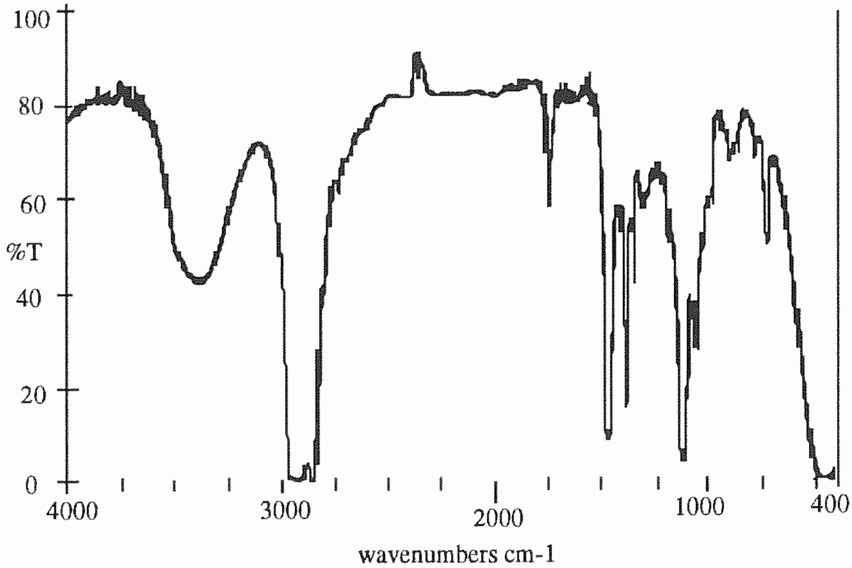


Figure 7.3 *Sec-pentyl-ethyl ether from DMSO*

In general, the students used excess bromoethane to make sure that all pentoxide would react. Since they knew about the decomposition of DMSO at high temperatures they did

not want to distil the crude product. They were still unfamiliar with vacuum distillation, and the time constraints did not allow for instructing the students on this technique. So instead, they tried to extract the ether by adding water. This initially did not result in phase separation. On my suggestion, they added an apolar solvent. A student asked me if diethyl ether would be okay. I agreed, but this choice soon proved unwise, since it made infrared analysis of the crude product useless. After that, I suggested to take pentane. This was distilled off afterwards, as was excess bromoethane. A final infrared spectrum of *sec*-pentyl-ethyl ether is reproduced in figure 7.3. Clearly visible is the ether absorption at 1120 cm^{-1}. The product also contained some *sec*-pentanol. The substance responsible for the absorption at 1720 cm^{-1} remained unidentified, although the wavelength suggests that it is a carboxylic compound. It probably stems from decomposition of DMSO.
In most cases, there was hardly enough time to complete the purification. The students definitely wanted to make the ether and complete the lab work, which implied that many things were discussed and executed in a hurry. As a result, I do not have high quality transcripts to display here. Evidently, the educational context of Ethers 2 still was too ambitious.

Another solvent available for sodium *tert*-pentoxide was ortho-xylene. The students had never heard of this substance, and they took for granted that this particular pentoxide could dissolve in it. In the course of the experiment, this variant was tried out by two students who had first, in vain, tried to achieve something with using alcohols and silver oxide. They decided to give it up and try the xylene variant that, until then, had not been used. However, gas chromatographic analysis initially showed no reaction in progress, too. They discussed this with me:

i6 Are we doing something wrong?
R What are you doing?
i6 Well .. we have that xylene .. with that tert-pentoxide in it .. but nothing happens.
R What did you do with it?
i8 We .. we just put it in the flask .. and then we put in that bromoethane .. and then we refluxed it. But it doesn't seem to do anything.
R So what are you going to do now?
i8 Well .. I think we should just wait a little bit longer, but she ..
i6 I was thinking .. can it be that it is steric hindrance? Ah .. how does that sodium-pentoxide dissolve? This .. xylene .. is that very polar?
R I think not.
i6 Well then .. is the sodium still on the pentoxide?
R You mean .. well .. I don't know. I can't see that. You see .. it is just a colourless liquid .. but .. maybe it is .. not ionized.
i6 But doesn't that mean that it can't react? We had that discussion .. about steric hindering and that .. if the sodium is still on the pentoxide .. maybe it cannot get at that bromo.
R Yeah ..?
i6 Well .. I have been looking at them .. they have that .. DMSO .. and that is also good .. it can dissolve it .. maybe .. when we use that too .. DMSO .. it can dissolve salts, can't it?
R Yes.
i6 Well .. if we just put in that DMSO .. maybe the sodium goes off .. and maybe it reacts.
R Hmm .. well .. that sounds plausible .. yes .. why don't you just try it? But .. watch out with that DMSO .. wear gloves .. and don't reflux .. cause it decomposes when it is too hot .. just gentle heating .. but good idea ..maybe it works.

Adding DMSO indeed had an effect on the reaction. Unfortunately, time was too short to work it all up and reach definite conclusions, but it seemed likely that the ether had been formed. The students were very satisfied with the chemical results. I was satisfied with the way they applied their understanding of structure-activity-relations to synthesis-planning in a way that fitted excellently in the simulation-of-research format.

7.11 Conclusion

In designing the educational context of Ethers I applied my understanding of the way students developed an understanding of organic synthesis in the educational context of Esters. With respect to synthesis-planning, esters achieved that students relate purification with formation. They learned to analyze the mass balance to determine the reaction-type. And they developed an understanding of structure-activity-relations which enabled them to apply an understanding of the Lewis representation of localized charges in ethers. They expanded their understanding of synthesis-planning to include the reaction medium. They learned a new reaction-type (the side-reaction). But they did not achieve an applicable understanding of the issue of delocalization. On the other hand, I noticed that a development of this understanding is necessary, since the students also failed to apply their textbook knowledge.

The format of simulation-of-research was sufficiently strong to enable students to act meaningfully and with purpose. However, students remained focused on the product of synthesis. They did not attain a theoretical viewpoint. Thus, in this context, they only applied what they already understood concerning structure-activity-relations instead of deliberately investigating questions regarding this issue.

I see three reasons for this. First, the educational context did not last long enough. Three four-hour lab periods apparently were too short to facilitate the necessary reflections and reapplications. Second, the TA's lacked the potential to guide students' attention to theoretical questions. Third, the educational context was not completely appropriate, since 'making the ether' remained the dominant point of view. The first to aspects can be remedied straightforwardly, by taking more time and by employing qualified TA's. The third aspect, I think, requires more research and probably a third expansion of the educational context. *If students can be brought into a context in which they investigate issues from a theoretical point of view, an context-specific integration of the situated aspects and the professional qualities of organic synthesis would be achieved.*

8 Discussion and conclusions

8.1 Summary

In this study, I attempted to study the relations between teaching and learning in education that aims at preparing students for doing research in organic synthesis. I discovered that current approaches to teaching this subject suffer from the so-called cookbook problem. In prescribed laboratory experiments, students appear to be able to produce the desired chemical results, but they do not achieve an understanding of the rationale of organic synthesis. Moreover, teaching, strictly speaking, does not explicitly aim at preparing students for doing research. It teaches students how to handle equipment, how to follow prescriptions, and how to reproduce well-known facts and explanations. Textbooks and curricular documents nevertheless suggest that students can learn to experiment in this way.

There can be no doubt that many students have achieved some competence in organic synthesis through this approach. However, this is something to be credited to the students themselves, and to ad hoc events during instruction. There is no explicit relation between teaching and learning. Since I wanted to study this relation, I had to develop an alternative educational format. I did not want to do this in an ad hoc manner. Hence, I also asked myself the question why it is that chemistry educators seem to think that providing students with facts and manuals also prepares them for doing research. I traced this down to an unwarranted application of objectivist philosophy to education. It seemed to me that a hermeneutic approach would be more suitable. I therefore analyzed the thought of the hermeneutic philosopher Hans-Georg Gadamer and applied his ideas to research in science education. Methodologically, this led to the hermeneutic research cycle. The hermeneutic cycle is a sequence of interpretation, understanding, and application, and applies as well to the chemical researcher, the student of chemistry, the teacher of chemistry, and the researcher of chemical education. My introduction of the hermeneutic cycle was in many ways an elaboration of what others, notably the participants in the WEI and my predecessors at the Department of Chemical Education at Utrecht University already applied.

From this theoretical viewpoint I further developed an interpretive methodology suitable for investigating my research question. Since this methodology is explicitly founded on hermeneutic principles and not on the objectivist paradigms it differs from many current approaches to research in science education.

I developed educational contexts in which students experienced and interpreted chemical phenomena in the context of organic synthesis, came to an understanding, and applied this in subsequent moments in the cycle. The educational contexts themselves were an application of my increasing understanding of the relations between teaching and learning. However, I could not investigate the hermeneutic cycle of the teacher.

The hermeneutic alternative to the prescription is the question. A question evokes attention to what is not yet understood. Questions generate viewpoints, discourse, hypotheses and experiences that can be interpreted. In order to generate the kind of questions and experiences that help prepare students for doing research in organic synthesis, an educational context of simulation-of-research had to be created. An important element in these contexts was what I called the issuing discourse, in which students interpreted and formulated their experiences in language, to reach mutual understanding of issues in organic synthesis.

In creating educational contexts I initially applied De Jager's synthesis-planning theory. I gradually realized that I also needed the concepts of reaction-type and of structure-activity-relations to meaningfully interpret students' developing understanding of organic synthesis.

Students achieved an understanding of the relation between reaction conditions and purification. They learned to apply an analysis of the mass balance to determine reaction-types. They could apply their understanding of the equilibrium reaction to synthesis-planning, and they also developed an understanding of the side-reaction. With respect to structure-activity-relations, students achieved an understanding of the Lewis formalism, which represents chemical properties in molecular structures using localized charges. An elaboration towards an understanding in terms of delocalized influences on stability and reactivity, succeeded only partially. This was related to the characteristics of the educational contexts I had created. These allowed the students to focus entirely on making the product. In this applied simulation-of-research context questions regarding theoretical issues did not lead to hypotheses and experiments to investigate these issues. In other words, further educational research could focus on the construction of contexts that help students to pose and investigate theoretical questions on structure-activity-relations. Such research could also elaborate on new reaction-types. An elaboration could also focus not only on batch syntheses but also on continuous synthesis processes as they occur in biosynthesis and in industry.

My investigations showed that students do not apply what they do not understand. This could have repercussions for the sequencing and the content of lecture courses and laboratory courses. Transfer of information seems appropriate only if students have acquired an understanding of the issues to be lectured on through experiences in the context from which such issues derive their meaning.

8.2 The teacher's cycle

When academic research is discussed, a theme that always comes up is the applicability in practice: "Nice work, Mr. Van Keulen, but what are we going to do with it?" I could hide behind the pretext that the results of academic work should have a fundamental, theoretical character instead of a direct applicability. After all, my basic research question was not to extinguish the cookbook problem or to develop a new curriculum in organic synthesis. Research at best clarifies problems; it does not solve them. Still, I think the results of my study could have important consequences for educational practice. However, the obvious, direct implementation of the educational contexts I developed into the curriculum, is not what I have in mind. Such a direct implementation would ignore the problems of understanding that occur in the teacher's cycle. In order to bring this point home, I describe in this section some of my experiences with an attempt at implementation.

After three cycles, I was satisfied with the research material I had gathered from Esters. So, in Esters 4, I shifted my attention from the students' understanding towards the teacher's understanding. Until now, I have paid little specific attention to the role of the teaching assistant. In previous chapters, I occasionally reported that I 'told the TA to ...'; I 'instructed the TA ..'; or I 'gave advise to the TA'. But I myself was always present to

influence the process. I occasionally asked questions to the students and I discussed the educational process with the TA, sometimes giving explicit advise. Consequently, the learning results I reported are not created entirely by a combined action of the manuals and the TA's teaching. In hermeneutic terms, the teacher's cycle was replaced by a combination of the TA and me. This combination developed and applied an understanding on how to teach in order to develop a specific student understanding. From the viewpoint of my research questions this suffices. But what would happen when I would not participate?
To answer this question, I used Esters 4 not only as a preparation for Ethers 2 but I also made an attempt to study the implementation into the lab course M&M1. To achieve this, Esters was treated as any other experiment in the course. The TA's were presented with a copy of the student manual and the teacher manual. I gave a ten-minute talk to introduce the experiment and explain my intentions, and then I retreated. The normal procedures were followed: the TA's read the texts and went to the lab to prepare themselves for those activities they did not feel familiar with. For example, most built a reflux apparatus, took some samples, and ran a few chromatograms.
I observed the actual execution from a distance, without participation. I did not talk to the students, nor gave advise whatsoever to the TA's. In order to generate some data I asked the TA's to tape-record their discussions with a portable tape recorder. My observations gave me a general idea of what the group was doing, whereas the tape recorders gave me some insight on questions concerning the development of understanding in this context.
I observed four TA's. One of them was a mature chemist with more than 15 years of experience with teaching lab courses. The other three had no teaching experience at all; one even had no research experience at all.

This last TA appeared to be very uncertain on how to organize the discussions and the lab work. He was extremely brief. The first discussion went as follows:

TA Well .. we are going to make esters. We are going to do it a little bit differently. First we are going to do those test tube experiments. Did you read that?
(silence)
TA Are there any questions?
(silence)
TA Okay, then you can start.

And that was it. The students went off to the lab to do the test tube experiments. They were having similar experiences as previous groups, and discussed these among each other. The TA, however, hardly showed up. During the second group discussion, he did not give much opportunity to discuss the experiences. He just asked what had happened, but did not comment on what the students said, nor did he ask for explanations or conclusions. Instead, he went on immediately:

TA We are now going to make the esters. For that .. you are going to reflux. You two.. are going to make methyl acetate and ethyl acetate .. you two are going to make methyl acetate and butyl acetate ..

Et cetera. He explained how to set up a reflux apparatus and how to draw samples for the gas chromatograph. So students set up the equipment, chose equimolecular amounts of alcohol and acetic acid, took samples, and ran chromatograms. In my opinion, they were

just doing what they were told to do, without asking questions, seeing any deeper points, or developing viewpoints. I noticed, however, that the students became aware of the fact that the alcohol did not disappear. They commented on this to each other, but the TA was not in the vicinity most of the time and missed these discussions.
After this stage, another very brief discussion took place in which the TA announced how to purify. He first asked the students how they wanted to purify, but got no immediate response to this direct question. Not knowing how to handle the situation, he just told the students working on ethyl acetate and methyl acetate to distil, and the students working on butyl acetate to wash and then distil. Thus, the students built a distillation apparatus. Most students observed very different boiling points than they had expected. This, I knew, was due to the formation of azeotropic mixtures. The TA apparently did not understand this issue, although I had written about it in the teacher manual. Indeed, I got the impression that he almost never consulted this manual. He ignored the distillation problems and told the students that everything was fine. The distillate was regarded to be the final, pure product. The TA thought it not necessary to analyze this any further and simply ended the experiment, without final group discussion.

My interpretation is that a TA without any teaching experience and with barely enough chemical experience to build a distillation apparatus has to assume such a teaching style. It masks his own uncertainty and preserves his authority. He was afraid to make mistakes and his solution for this was to avoid everything that could raise problems he could not handle. He did not ask questions because he knew he could not provide some of the answers himself. In an objectivist framework, not knowing the correct answers is the same as lack of understanding. It is clear that a TA wants to avoid giving this impression.
Although I was not very happy with what happened, it is not my intention to put the blame on the TA. According to my own standards he was not prepared properly for the task. But the development of such a proper preparation could benefit from the experiences of these underprepared TA's.

A second TA also was unexperienced and uncertain, but performed quite differently. He was afraid to take decisions. This TA also had difficulty to lead discussions and to ask relevant questions. He listened, but he could not bring the students to make choices. As a result, discussions went on endlessly, often without any direction or conclusion. The same happened in the laboratory. The students went on refluxing and taking chromatograms for hours, although no significant change was monitored anymore. The consequence was that they did not finish within the time limit, and the experiment had to be ended prematurely.

At M&M1, it is not uncommon for TA's to occasionally exchange with another TA, often for personal reasons. This is what happened to my third TA. He led the first group discussion and the test tube experiments, but then had some other obligations. So the next morning a substitute showed up, much to my surprise. This TA did not know Esters, did not have the manuals, and also was rather surprised. However, he had some talent for teaching. He had the students have their way and was as curious as they about what would happen. He, however, did not know much about gas chromatography, nor about distillation, so the group's progress was hampered by many unnecessary practical problems. Since this group had to figure out what to do by themselves, animated and relevant discussions on the phenomena under consideration took place. But the TA was not able to give a structure to this process and to turn experiences into explicated understanding.

The following is a description of discourse that is almost the contrary of what I intended. The discourse was led by a TA who knew all about esterification, equilibrium, gas chromatography and distillation, and had been teaching lab courses for many years. He apparently applied the (objectivist) teaching style he had grown accustomed to. He made sure that the students went through the intended experiences, but he explicated almost everything himself. The next transcript is illustrative for this style:

TA Now you have refluxed and analyzed the samples with the gas chromatograph. This is the reaction: [writes on the blackboard]

$$\text{alcohol} + \text{acid} \rightarrow \text{ester} + \text{water}$$

TA Well, what is in the reaction mixture?

s1 Alcohol and ester.

TA Yes, because it actually is an equilibrium [changes the arrow on the blackboard into equilibrium arrows]. From the ratio of alcohol and ester you can determine how the equilibrium is. Which ratio of alcohol to acetic acid did you take?

s2 Well .. simply .. 1 to 1.

s3 We took two times as much acetic acid.

TA Yes, that is very clever, because in that case you end with less alcohol. Let us take a look at the table in the manual, with the physical constants. How do you actually want to purify? Look to the list of boiling points.

s4 Distillation.

TA Which product do you have?

s4 Ethyl acetate.

TA That could prove to be difficult. Maybe it is possible with a Vigreux column. It is very difficult when the boiling points of substances are so close to each other. (..) If the boiling points do not differ enough then you can't distil. What you could try to do is washing with water. In this case, if you have used excess acid, then the alcohol is already gone. So you don't need to distil to separate ethanol from ethyl acetate. But you still have acetic acid, since that was present in excess. You could wash that. But: ethyl acetate dissolves a little bit in water, so I shouldn't use too much water. You would lose too much product. Washing is something we do with a separation funnel. I'll show you that later. (..) And what are we then going to do with the ethyl acetate? It will always contain water. We can remove that with a drying agent. That is a salt that binds to water very well. For example magnesium sulphate. Look, that is in that jar over there. And do you think it will then be 100% pure ethyl acetate?

s5 No.

TA No. And how are we going to do the final purification?

(silence)

TA Now we can distil. So the sequence is: first washing with water, then drying, and then distilling. Now methyl acetate. Can you wash that with water?

s2 No, it dissolves in water.

TA No, you'd lose everything.

s4 Distillation.

TA Yes, that is a possibility. (..) I would use a Vigreux column in that case. The difference in boiling point between methanol and methyl acetate is less than 10 degrees. And butyl acetate?

s3 Same as with ethyl acetate.

TA Yes, you can wash that, because butyl acetate does not dissolve in water. But butanol?

s1 Doesn't either.

TA Yes. But if I had taken a nice excess of acid, what would have happened to the alcohol?

s4 Would be gone completely.
TA Yes.

Needless to say that this group obtained excellent chemical results and had no problems with the time limit. However, according to hermeneutics, understanding is a process, in which it is necessary that the participants take their own viewpoints, interpret, choose and act accordingly, and formulate their experiences in their own words. This, as well as the simulation-of-research format, is violated. Transfer of objective knowledge does not lead to understanding. I am afraid that this teaching style just leads to chemical results at the expense of developing understanding.

There can be only one conclusion: implementation in the present curricular context does not lead to the intended outcomes. Students in all groups, regardless of the TA, certainly learned a few things from the experiment, but more opportunities were missed. A reproducible relation between teaching and learning was not achieved. I think that I did achieve such a relation in the educational contexts I described previously. In my opinion, it must be possible to achieve good teaching results even with inexperienced TA's if three conditions are met. First, TA's should be able to listen, to ask questions, and to guide decision making. Second, there should be sufficient time to constitute experiences and issuing discourse during pre-service teacher education. Third, in-service teacher education could be included. This could have the form of participation of and interaction with a more experienced teacher during the experiments. TA's should be given the opportunity to learn, to reflect on their teaching, and to reapply their understanding in a subsequent cycle. At M&M1, none of these conditions could be met, and I am afraid this is typical for lab courses that use the prescription format.

I conclude that implementation cannot be achieved by simply handing out student and teacher manuals. For that reason, I did not include these texts, say, as appendices to this study. Application takes an understanding of the intended educational contexts, an understanding that cannot be achieved by transfer of the information. I assume that chemistry teachers who understand are able to apply the results of my study in their own educational contexts, if they wish to do so.

8.3 A future for a hermeneutic approach?

Unfortunately, my results run counter with the current situation in chemistry education. Developments also point in the reverse direction. Due to recent budget problems, universities in The Netherlands were forced to reduce their curricula considerably. Also, scholarships were reduced, which ensured that the average student completes his or her studies at a faster pace, at a younger age, and without much academic or research experience. At the same time, TA's became less experienced and stayed for a shorter period, too. All these factors contributed to the cookbook character of the laboratory course. In an attempt not to lose too much content the curriculum became more scholastic. Laboratory work, which is expensive with respect to both time and money, lost some extent and the organization became stricter.

To cope with less experienced TA's and with severe time constraints, the lab course management introduced more sophisticated equipment that would enable to do the same experiments in less time and with more reliable results. Chromatographs were equipped with automated integrators, glass burettes were replaced by automated ones with digital displays, etc. Also, the manuals, especially the teacher manuals, grew ever more detailed. In the words of the director of the lab course: "We have to make the experiments teacher-proof". That is, TA's lack understanding, will never attain understanding during their stay as TA, and hence, have to follow a recipe. In this way, the students can obtain approximately the same chemical results as ever, but in my opinion this is achieved at the expense of more valuable learning results.

There is little that a Faculty of Chemistry in The Netherlands can do about government budget problems, reduced scholarships, and government imposed reduced curricula. However, there is some freedom of choice regarding the internal organization. One could decide to pay more attention to the quality of teaching. At M&M1, TA's are not recruited or selected by the management team, but they are sent by the various Departments. It is normal for a Department to send to a lab course those members that are its least valuable researchers, which means, on average, the youngest and chemically least experienced. Or, if they have the money, they can hire an even less experienced student to do the job. Since the application of the objectivist framework to teaching suggests that understanding is not required, there is little incentive for Departments to change this attitude.

The lab course's organization of fixed experiments with fixed prescriptions also does not take advantage of whatever special qualities a TA might have. Even when a TA is good organic chemist or a good teacher, he or she still has to follow the same prescriptions. This does not contribute much to the TA's personal or intellectual commitment to the lab course.

My approach to education suggests a different organization. TA's should have an understanding of chemistry and of research; they also should have or acquire experience with teaching, especially with listening, observing, and leading issuing discourse. The best would be to let teacher's participate in the construction of educational contexts that simulate the research area with which they are acquainted. In that way, their own research could benefit from their teaching efforts, because the act of teaching requires the explication of tacit understanding.

This suggestion appears to be expensive. Developing educational contexts through the hermeneutic cycle approach requires time and attention. Experienced teachers are more expensive too. On the other hand, it is no longer necessary to have students move through a collection of randomly selected prescriptions in order to illustrate all the techniques, reactions and substances of organic chemistry. This is expensive too, and it hardly prepares students for doing research. The 'minds-off' prescription approach does not require that teachers interpret and reflect for themselves because all the answers are known in advance. A change towards a hermeneutic approach appears to require more effort. But it leads to applicable learning results that are explicitly known, instead of ineffective, ad hoc and implicit. The quality of the learning results can be raised, which makes teaching more effective and hence more efficient. If chemistry teaching is to keep up with current developments in research and society, a hermeneutic approach will be rewarding.

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Samenvatting

Dit proefschrift beschrijft een onderzoek dat plaatsvond in de vijf jaar tussen 1990 en 1995 aan de Faculteit Scheikunde van de Universiteit Utrecht. Ik heb daar een *chemiedidactisch* onderzoek uitgevoerd naar het leren en het onderwijzen van de organische chemie. Chemiedidactiek onderzoekt scheikunde-onderwijs en stelt daarbij de vakinhoud centraal. Hoe moet, in onderwijssituaties, dat wat chemici weten en kunnen gestruktureerd worden zodat ook studenten tot bruikbare kennis en inzichten komen? Het gaat dus om de relaties tussen onderwijzen en leren: wat is het precies in wat de docent zegt of wat het tekstboek schrijft, dat er toe leidt dat studenten chemie gaan begrijpen? Is het mogelijk om een chemiedidactische theorie te ontwikkelen die dit proces zelf begrijpelijk maakt?
Chemiedidactiek heeft natuurlijk raakvlakken met andere disciplines die het onderwijs onderzoeken. Maar er worden andere accenten gelegd. Het gaat niet in de eerste plaats om de groei naar volwassenheid, zoals in de pedagogiek, of om de werking van mentale processen, zoals in de psychologie. Volwassenheid en psychologische begrippen zoals intelligentie vallen niet samen met het vermogen om chemisch onderzoek te doen. Algemene onderwijskundige theorieën zijn niet zonder meer toepasbaar op specifieke vakinhouden en vakcontexten.
Scheikunde staat bij velen bekend als een moeilijk vak. Scheikundige competentie is niet aangeboren, je leert het niet door opvoeding of op straat, het is eigenlijk alleen via onderwijs te verwerven. Daarom is het belangrijk dat het scheikunde-onderwijs voldoende hulp biedt. De studie scheikunde bereidt studenten voor op het zelfstandig doen van wetenschappelijk scheikundig onderzoek. Dit doel wordt nagestreefd door studenten allerlei studie-onderdelen te laten volgen. Als het goed is beïnvloeden die studie-onderdelen het leren van de studenten daadwerkelijk in de gewenste richting. Pas dan is er een zinvolle relatie tussen het leren en het onderwijzen, en pas dan heeft het zin om die relatie te onderzoeken.

In hoofdstuk 2 ga ik daarom na wat de bestaande relatie is tussen leren en onderwijzen. Daarbij heb ik mij vooral gericht op het practicum voor eerstejaars scheikundestudenten Meten & Maken 1, en daarin op het onderwerp organische synthese. Om die relatie in kaart te brengen ga ik na wat de doelen zouden moeten zijn voor onderwijs dat voorbereidt op het doen van onderzoek. Ik ga er dus niet voetstoots van uit dat het bestaande onderwijsprogramma (het 'curriculum') aan alle eisen voldoet. Daarom analyseer ik het kritisch. Niet met kwade bedoelingen, om te laten zien dat er niets van deugt. Maar om na te gaan of ik mijn, nogal specifieke, onderzoeksvraag kan beantwoorden: bereidt het onderwijs in de organische chemie de studenten expliciet voor op het doen van wetenschappelijk onderzoek?

Daarbij lijkt het mij vanzelfsprekend, dat de normen daarvoor uit de praktijk komen. Welke eigenschappen hebben professionele organisch chemici die hen in staat stellen om succesvol onderzoek te doen? In mijn analyse laat ik zien dat chemici beschikken over datgene wat vaak met 'kennis en vaardigheden' wordt aangeduid: ze kennen de feiten, modellen, en theorieën, en ze kunnen in het laboratorium de instrumenten bedienen en de experimenten uitvoeren. Maar minstens zo belangrijk is dat ze hun werk niet in isolement doen: er is ook altijd een onderzoeksprogramma met heel specifieke onderzoeksvragen, en er zijn collega's waarmee tot overeenstemming gekomen moet worden over de interpretatie van de resultaten. Experimenten worden uit theorieën en hypotheses afgeleidt, en experimentele gegevens zetten aan tot nieuwe theorievorming. Zo zijn theorie en praktijk altijd aan elkaar gekoppeld en geven ze elkaar betekenis.

In het curriculum is hier echter weinig van terug te vinden. In de officiële curriculumdocumenten wordt weliswaar als belangrijk doel aangegeven dat de studenten moeten 'leren experimenteren', maar in de praktijk komt daar niet zoveel van terecht. Dat komt omdat er, bewust of onbewust, eigenlijk een heel ander doel wordt nagestreefd: het onderwijs moet een representatief beeld geven van de huidige chemische kennis en laboratoriumtechnieken. Daartoe is een scheiding gemaakt tussen college en practicum: in het college ('theorie') worden de feiten (de stofklassen, de reakties, de reaktiemechanismen) meegedeeld, en in het practicum ('praktijk') worden de technieken geoefend.
Daarbij gaat het niet echt om 'leren experimenteren', maar hooguit om 'leren voorschriften uit te voeren'. Het verband tussen theorie en praktijk is weg. De reden om een bepaalde techniek, bijvoorbeeld een destillatie, uit te voeren is niet omdat zo een bepaalde vraag beantwoord kan worden, soms zelfs niet eens om een mengsel daadwerkelijk te zuiveren, maar om de studenten te leren hoe ze een destillatie-opstelling moeten bouwen en een destillatie moeten uitvoeren. Dat is nuttig, maar het is niet voldoende voor onderwijs dat voorbereidt op het doen van wetenschappelijk onderzoek.
Men spreekt in de literatuur dan ook wel van een 'kookboekprobleem': studenten voeren (soms heel ingewikkelde) voorschriften uit, bereiken daarmee chemisch gezien goede resultaten, maar ze begrijpen niet goed wat ze doen. Ik heb daar een detail-studie naar gedaan. Op het practicum wordt al heel lang via een voorschrift aspirine gemaakt. De studenten slagen er heel goed in om die aspirine te maken, maar de redenen om de dingen te doen zoals ze in het voorschrift staan worden niet begrepen. Ja, ze hebben dat begrip helemaal niet nodig, omdat alles al heel duidelijk in het voorschrift staat. In synthese-experimenten worden stoffen gemaakt, terwijl het eigenlijk de bedoeling is dat studenten verstandig gemaakt worden.
Ik ben niet de eerste die daar op wijst. Ik analyseer daarom ook allerlei bestaande suggesties om het kookboekprobleem op te lossen, maar die bevredigen mij niet erg. Meestal blijven in het onderwijs voorschriften centraal staan. Een groot probleem is dat, hoewel de studenten ongetwijfeld het een en ander leren van voorschriftproeven, er geen duidelijk aanwijsbare bijdrage is van het onderwijs wanneer het gaat om het leerdoel 'leren experimenteren'. De relatie, als die er al is, is impliciet en laat veel (te veel) aan de student over. "De goeden komen er uiteindelijk wel", wordt wel eens gezegd. Dat is waar, maar ik vind dat onderwijs daarbij behulpzaam moet zijn, en dat ook de wat minder goeden het vak kunnen leren. Bovendien is chemie een cumulatieve wetenschap: er komt steeds meer bij wat om een illustratie vraagt. Zonder een selektiecriterium zouden studenten eigenlijk een ongelimiteerd aantal illustratieve proeven moeten uitvoeren, wat bijzonder inefficiënt is. En ook dan ontbreekt nog de relatie tussen theorie en praktijk.
Het probleem, zoals ik dat zie, is dat veel chemiedocenten en ontwerpers van curricula kennelijk denken dat het mogelijk is onderdelen van de chemie (de feiten, de technieken) afzonderlijk te trainen, waarna dan 'vanzelf' een integratie optreedt waarbij studenten 'begrijpen', en hun kennis en vaardigheden kunnen toepassen in onderzoek.

In hoofdstuk 3 ga ik daarom dieper in op het probleem van het begrijpen. Ik zie dat eerstejaars scheikundestudenten behoorlijk veel kennis moeten hebben. Ze zijn in staat een voldoende te halen voor het tentamen organische chemie, en ze slagen er ook in om alle organische synthese-proeven met succes uit te voeren. Ze leren diverse apparaten bedienen en verwerven zich allerlei nuttige laboratoriumvaardigheden. Toch is dit niet hetzelfde als 'begrijpen'. Dan zouden de studenten immers in staat moeten zijn om samenhangen te zien en de kennis die ze hebben moeten kunnen toepassen in nieuwe situaties. En dat blijkt niet zo te zijn.

Voor veel chemici is dat verwarrend. Immers, zij hebben hun vakgebied goed en geordend in hun hoofd zitten. Chemie kan worden onderverdeeld in een aantal terreinen, zoals organische chemie, anorganische chemie, biochemie, thermodynamica, etc. Daarbinnen kan de kennis verder worden geclassificeerd: er zijn in de organische chemie allerlei stofklassen, reaktietypen, en mechanismen. Ook zijn er een aantal voor de organische chemie belangrijke laboratoriumtechnieken. Wie daarvan kennis heeft weet wat er te weten valt, en moet dat kunnen toepassen, vinden velen. Wat valt er verder nog te begrijpen? De natuur zit immers zo in elkaar? Dus is het onderwijs vooral een kwestie van alles goed uitleggen en overdragen, en goed oefenen.

Ik denk dat hier op een onbewuste en misschien onbedoelde wijze een bepaalde filosofie in het onderwijs binnensluipt. Ik duid die filosofie aan met 'objectivisme'. Het objectivisme stelt dat de wereld bestaat uit entiteiten ('dingen'), die bepaalde eigenschappen hebben en op bepaalde manieren met elkaar samenhangen. Zo is er een aarde, en die is rond. Bovendien is het een planeet, en geen ster. Scheikunde gaat over stoffen, maar die stoffen zijn eigenlijk opgebouwd uit atomen, die met elkaar verbonden zijn tot bijvoorbeeld molekuulstructuren.

Nu gaat het mij er niet om deze filosofie te bestrijden. Waar het mij wel om gaat is dat de gedachtenloze toepassing in onderwijs tot problemen kan leiden. Het overdragen van kennis en het oefenen van technieken leidt er niet zonder meer toe dat de studenten onderzoeksvaardig worden. Dat komt omdat vergeten wordt dat elk feit een antwoord is op een (onderzoeks)vraag. Studenten leren wel de antwoorden, maar ze leren niet om vragen te stellen. Daardoor kunnen ze een feit ook niet zien als een antwoord op een vraag, en is er geen sprake van toepasbare kennis. Het blijft steken in een geïnformeerd zijn.

Ik zoek daarom naar een theoretisch kader dat meer recht doet aan wetenschap als een proces van vraag en antwoord. Ik sluit daartoe aan bij denkbeelden van een aantal Nederlandse chemiedidactici die bekend staan onder de naam Werkgroep Empirische Inleiding. Tegelijk probeer ik hun ideeën van een fundament te voorzien. Ik vind dat fundament in de filosofische stromingen van de fenomenologie en vooral in de hermeneutiek, met name zoals beschreven door Hans-Georg Gadamer. Het uitgangspunt hierin is niet dat er een wereld bestaat gevuld met objecten. Dat wordt niet ontkend, maar de kennis die mensen hebben van de objecten komt altijd via ervaringen en interpretaties tot stand. Objecten, en daarmee ook wetenschappelijke feiten worden geconstitueerd door ervaring, interpretatie en consensus. Dat betekent dat de wijze waarop 'iets', bijvoorbeeld een chemische reaktie, ervaren wordt van invloed is op de interpretatie van het fenomeen. Dit wordt in de hermeneutiek beschreven met de termen 'gezichtspunt' en 'context'. Iedereen, ook de chemisch onderzoeker, de student scheikunde, en de chemiedidactisch onderzoeker beschouwt wat zich opdringt vanuit een bepaald gezichtspunt, met bepaalde verwachtingen en vanuit specifieke vooronderstellingen. Die bepalen de betekenis van wat

ervaren wordt. Zo kan een zaak vanuit verschillende gezichtspunten 'begrepen' worden. De kwaliteit van het begrijpen blijkt uit de toepassing, uit het vermogen om scherper te interpreteren en betere vragen te stellen. Er is daarmee een eenheid van interpreteren, begrijpen en toepassen. De taal speelt een belangrijke rol: ervaringen moeten onder woorden worden gebracht, en er moet ook consensus ontstaan over de interpretaties. Anders gaat het niet om wetenschappelijke kennis, maar om persoonlijke overtuigingen.
Hoewel dit kader allereerst in de geesteswetenschappen is ontwikkeld, bijvoorbeeld bij de interpretatie van oude teksten, is het mijns inziens ook van toepassing op de natuurwetenschappen. Ook daar wordt geïnterpreteerd, begrepen en toegepast. Het doel van de natuurwetenschappen is het verkrijgen van objectieve kennis, omdat daarmee voorspeld en beheersd kan worden. De natuurwetenschap wil graag uitspraken doen die algemeen geldig zijn, en niet alleen hier en nu en voor bepaalde mensen in een specifieke situatie. De resultaten van het scheikundig onderzoek, zoals weergegeven met behulp van atomen, molekulen, en reakties, hebben daardoor een tijdloos, ahistorisch karakter. Een reaktie is pas volkomen beheersbaar als alle tijdgebonden en toevallige factoren uitgeschakeld zijn. Een molekuul staat niet in onze tijd, heeft geen geschiedenis. Per definitie is het ene molekuul H_2O gelijk aan het andere.
'Begrijpen' echter is wel altijd gebonden aan tijd en context. Het is niet mogelijk jezelf bij de haren op te tillen om eens te kijken hoe het echt zit. We moeten het doen met contextgebonden ervaringen en interpretaties, en daarover moeten we het met elkaar eens zien te worden. Dat is onze geworpenheid, om het met de filosoof Heidegger te zeggen. Dit moet mijns inziens consequenties hebben voor onderwijs. Immers, je kunt studenten wel vertellen wat de huidige stand van zaken in de wetenschap is, maar als zij niet bekend zijn met de context die verantwoordelijk is voor de betekenis van de gebruikte vaktermen en handelingen, dan zullen zij ze niet op dezelfde manier begrijpen als de wetenschappers die deze feiten, theorieën en processen ontwikkeld hebben en gebruiken. En daarmee wordt twijfelachtig of de studenten in staat zullen zijn hun kennis toe te passen.

Op basis van deze analyses probeer ik in hoofdstuk 4 een methodologie te ontwikkelen om dit proces van begrijpen te bestuderen. Ik analyseer een aantal bestaande methoden, maar constateer dat nogal wat onderwijsonderzoek geënt is op het objectivisme. Ik zoek naar een methode die mij in staat stelt te onderzoeken hoe studenten tot een begrip van de chemie komen. De methode die ik ontwikkel komt neer op een cyclisch proces van interpreteren, begrijpen en toepassen, dat zowel voor mij als onderzoeker geldt als voor de studenten. Ik wil daartoe een onderwijscontext ontwerpen waarin studenten chemische ervaringen kunnen opdoen en die interpreteren. Op basis daarvan zullen ze in gesprek moeten raken om met elkaar tot consensus te komen. Daarbij wordt hun begrijpen onder woorden gebracht, en voor mij onderzoekbaar. De studenten kunnen hun begrip daarna toepassen in de chemische context door hypotheses te formuleren en experimenten op te zetten. Ook dat is iets waar ik onderzoek aan kan doen. Voor mij geldt dat ik interpreteer wat er precies in die onderwijscontext gebeurt, dat wil zeggen, ik probeer het handelen en het spreken van de studenten te begrijpen en dat in chemiedidactische begrippen formuleer. Ik pas mijn eigen begrijpen toe door de onderwijscontext met behulp van die begrippen verder te ontwikkelen. Zo hoop ik in enkele cycli te komen tot een onderwijscontext waarin onderwijzen en leren aanwijsbaar en produktief gekoppeld zijn.

Mijn voornaamste onderzoekstechnieken zijn het observeren van onderwijsprocessen en het op band opnemen en analyseren van de gesprekken die de studenten met elkaar en met hun docenten voeren. Ik geef daar in dit proefschrift vele voorbeelden van.

In hoofdstuk 5 en 6 beschrijf ik hoe ik via zo'n cyclisch proces tot een effektieve onderwijscontext ben gekomen. Ik gebruik met opzet niet het woord 'experiment', of 'proef', omdat dat teveel aan de bekende kookboekvoorschriften doet denken. Waar het mij omgaat is de combinatie van experimenteren en argumenteren (waaronder ook het uitvoeren van berekeningen valt) die kenmerkend is voor onderzoek, maar die juist zo zelden voorkomt in het onderwijs. Ik noem deze 'werkvorm' *simulatie-van-onderzoek.* Het gaat er niet om dat studenten werkelijk zelf nieuw onderzoek doen, maar dat de kenmerken van onderzoek aanwezig zijn: een zich opdringende verwondering over een verschijnsel, de herkenning dat een onderdeel van de chemie daar iets zinvols over kan zeggen, het stellen van gerichte vragen, het formuleren van hypotheses, het bedenken en uitvoeren van experimenten die de vragen zouden kunnen beantwoorden, het interpreteren van de empirische gegevens, het bijstellen van de hypotheses en vooronderstellingen, en zo in een cyclisch proces steeds verder. Daarbij gaat het er in onderwijs om dat zodanige chemische verschijnselen gekozen en gepresenteerd worden dat de studenten als groep hun begrip kunnen uitbreiden en verdiepen.

De chemische context in deze hoofdstukken betreft het maken van esters. In plaats van studenten een voorschrift te geven confronteer ik ze met een vraag: Hoe kun je esters maken? Studenten denken dat te weten, namelijk door een alcohol en een carbonzuur bij elkaar te voegen. Er is dus een uitgangspunt om te experimenteren. Ik laat de studenten hun idee uitvoeren, en daarbij doen ze allerlei ervaringen op. Zo nemen ze waar dat, wanneer je twee kleurloze vloeistoffen bij elkaar doet met de bedoeling een andere kleurloze vloeistof te maken, er eigenlijk niet zo veel van dat proces te zien is. Treedt er wel een reaktie op? Uit de waarneming dat sommige reaktiemengsels na verloop van tijd een zoete geur verkrijgen kan dit worden afgeleid. Maar het proces gaat niet overal even snel: een mengsel van butanol met mierezuur ontwikkelt aanmerkelijk sneller een zoete geur dan een mengsel van methanol met azijnzuur. Hoe komt dit? Ik laat de studenten hun waarnemingen rapporteren en bediscussiëren. In dergelijke gesprekken wordt soms consensus bereikt over interpretaties. Ook worden nieuwe problemen en hypotheses onder woorden gebracht, wat aanleiding geeft tot nieuwe experimenten.

Nu gaat het er mij niet in de eerste plaats om dat de studenten uiteindelijk zuivere esters gesynthetiseerd hebben. Een dergelijk resultaat wordt ook bereikt, maar veel belangrijker vind ik dat de studenten leren begrijpen waar het in de organische synthese op aan komt. Ik laat zien hoe ik zelf in een cyclisch proces van interpreteren, begrijpen en toepassen op het spoor ben geraakt van een aantal chemiedidactische thema's die het leren begrijpen van organische synthese struktuur bieden.

Het eerste thema, *syntheseplanning*, is een verdieping van eerder onderzoeksresultaat van De Jager (1985). In dit kader moeten studenten leren begrijpen dat een synthese bestaat uit een aantal stappen die relaties met elkaar hebben. Een voorbeeld: ethanol en ethylacetaat hebben fysische eigenschappen die weinig van elkaar verschillen, zoals hun kookpunt en oplosbaarheid. Wie ethylacetaat wil maken uit ethanol en azijnzuur zal dus moeten voorkomen dat het ruwe product nog veel ethanol bevat, aangezien ethanol heel moeilijk te verwijderen is. Een goede oplossing is om in de vormingsstap een overmaat azijnzuur te gebruiken. Dus in de vormingsstap moet rekening gehouden worden met de zuiveringsstap. Wie aan dergelijke dingen denkt zonder dat iets voorgeschreven wordt heeft inzicht in syntheseplanning. Studenten leggen deze koppeling niet meteen. Door het interpreteren, begrijpen en onderzoeken van hun eigen chemische ervaringen ontwikkelen ze dit inzicht. Een op deze wijze ontwikkeld inzicht is vervolgens ook toepasbaar in andere contexten.

Het tweede thema waarvan ik het grote belang ontdekte, is het thema *reaktie-type*. Het spreken en handelen van studenten lijkt vaak gebaseerd te zijn op de impliciete veronderstelling dat reacties van het type A + B → C zijn. Dat wil zeggen, je doet de uitgangsstoffen bij elkaar, er vindt reaktie plaats, en na afloop heb je het produkt over. Zo'n ideaal-typische reaktie komt echter in de praktijk niet voor. Niet alleen zullen er altijd resten uitgangsstof aanwezig zijn (A en/of B), maar ook onstaat er vaak een bijprodukt (D). Daarnaast bestaan er ook andere reaktie-typen, zoals de evenwichtsreaktie en de nevenreaktie. Het is in het onderwijs gebruikelijk om dergelijke informatie vooraf aan studenten mee te delen. Inderdaad zijn er studenten die desgevraagd kunnen melden dat de veresteringsreaktie een evenwichtsreaktie is. Het cruciale punt is dat ook deze studenten, als niemand hen vertelt wat ze moeten doen, er in hun praktijkbeslissingen geen rekening mee houden. Om kennis toe te passen moet je het niet alleen kunnen reproduceren op tentamens, je moet het ook begrijpen. Daartoe moet kennis een resultaat zijn van eigen ervaringen in een chemisch relevante context.

De veresteringsreaktie vormt zo'n context, omdat zich een evenwicht instelt waarbij twee produkten (ester en water) in evenwicht zijn met twee uitgangsstoffen (alcohol en carbonzuur). Dit kan afgeleid worden uit een bepaling van de hoeveelheden en de identiteiten van de stoffen in een mengsel (de stofbalans) op verschillende momenten gedurende de synthese. Maar dan moet je wel oog voor deze zaak hebben. In de onderwijscontext wordt de aandacht van de studenten daarop gericht, doordat ze, wanneer ze hun synthese beginnen met gelijke hoeveelheden alcohol en carbonzuur, een hoeveelheid alcohol overhouden waar ze niet door zuivering van af kunnen komen. Door over deze ervaringen na te denken en met elkaar te spreken begrijpen ze dat ze die hoeveelheid alcohol kunnen terugdringen door de synthese met een overmaat carbonzuur uit te voeren. Zo is dit theoretisch thema reaktietype toepasbaar bij het nemen van praktijkbeslissingen in het kader van syntheseplanning. Immers, de overmaat carbonzuur is gemakkelijker te verwijderen dan een klein restant alcohol.

Het derde thema dat in de organische synthese belangrijk is, betreft de *struktuur-aktiviteitsrelaties*. In wetenschappelijk verband worden syntheses niet uitsluitend uitgevoerd om bepaalde nuttige of nieuwe produkten te maken, maar ook om zo een dieper theoretisch inzicht te verwerven in de eigenschappen van stoffen. Zo is een eigenschap (of: aktiviteit) van alcoholen dat ze met carbonzuren tot esters reageren. Maar waarom eigenlijk? Is het mogelijk om dat aan de stof te 'zien'? Chemici kunnen dergelijke stofeigenschappen niet zonder meer herkennen aan de makroskopische stof als zodanig. Maar ze kunnen wel proberen belangrijke eigenschappen af te beelden in een representatie: bijvoorbeeld met een brutoformule of een struktuurformule. Zo beeldt de formule CH_3CH_2OH een aantal eigenschappen van de stof ethanol af. De chemicus kan aan de aanwezigheid van de OH-groep herkennen dat deze stof met carbonzuur tot ester kan reageren. Ik laat in mijn onderzoek zien dat studenten niet zonder meer in staat zijn op deze wijze struktuur-aktiviteitsrelaties te leggen, te herkennen of te onderzoeken. In eerste instantie herkennen ze in de OH-groep geen chemische eigenschappen. Ze zien het als een label, een soort naamkaartje waaraan je kunt zien dat deze stof een alcohol is. Ook moeten

ze leren dat de twee zuurstofatomen in azijnzuur (CH_3COOH) niet gelijk zijn, en ook weer anders dan het zuurstofatoom in ethanol. Azijnzuur staat weliswaar vanwege zijn vermogen om een proton af te staan bekend als een zuur, maar de zuurstofatomen kunnen met hun vrije elektronenparen ook een waterstofatoom accepteren. Chemici spreken dan van een Lewis-base. Studenten herkennen zulke eigenschappen niet zomaar aan een struktuurformule. Dat moet geleerd worden. Specieker: ze moeten leren begrijpen dat chemische eigenschappen gerepresenteerd kunnen worden met behulp van gelokaliseerde lading, bijvoorbeeld een elektronenpaar op zuurstof ($\delta-$) of een klein tekort aan lading op een bepaald koolstofatoom ($\delta+$). Pas dan kunnen ze begrijpen dat ethanol met azijnzuur reageert, en de zo ontwikkelde struktuur-aktiviteitsrelatie toepassen op andere stoffen.
Ik laat gedetailleerd zien hoe ik deze thema's in nieuwe onderzoekscycli verwerkt heb. De onderwijscontext wordt daardoor steeds produktiever: studenten slagen er steeds beter in inzicht te verwerven in de organisch-chemische thema's. Ik laat dat zien aan de hand van gedetailleerde fragmenten van gesprekken tussen studenten onderling en met hun practicumdocent. Na enkele cycli ben ik vrij goed in staat om op een kwalitatieve wijze te voorspellen hoe het onderwijsproces zich gaat voltrekken. Dat stelt mij ook in de gelegenheid de docenten te informeren over de manier waarop studenten tot begrijpen komen.

In hoofdstuk 7 bouw ik voort op het bereikte door een nieuwe onderwijscontext te maken, Ethers genaamd. Ik pas daarin mijn eigen begrijpen toe door de context van de drie thema's uit te breiden op punten waarvan ik vermoed dat het begrijpen van de studenten verder ontwikkeld moet worden. Ik kies opnieuw voor simulatie-van-onderzoek: geen voorschrift, wel een startvraag. In dit geval is de chemische context de synthese van een drietal asymmetrische ethers: n-pentyl-ethyl ether, sec-pentyl-ethyl ether, en tert-pentyl-ethyl ether. Asymmetrische ethers worden vaak gemaakt via de zogenoemde Williamson ether synthese: een halogeenalkaan (bijvoorbeeld broompentaan) reageert met een metaal-alkoxide (bijvoorbeeld natriumethoxide). Het mechanisme van die reaktie is een nukleofiele substitutie van de tweede orde. Deze reaktie kan worden voorgesteld door een gelokaliseerde negatieve lading op het zuurstofatoom van het ethoxide aan te laten grijpen op dat koolstofatoom van het halogeenalkaan dat verbonden is met het halogenide. Ik veronderstel dat de studenten een dergelijk mechanisme nu kunnen begrijpen, omdat ze deze struktuur-aktiviteitsrelatie in de vorige onderwijscontext geleerd hebben. Ik schrijf dan ook niet de uitgangsstoffen van de reakties voor. De studenten moeten nu in staat zijn een beredeneerde keuze te doen, en beginnen zo een nieuw proces van experimenteren en argumenteren.
Ik ga ervan uit dat de studenten de genoemde thema's nog niet volledig begrijpen. Met betrekking tot het thema reaktietype hebben ze weliswaar de evenwichtsreaktie leren begrijpen, maar nog niet de nevenreaktie: de mogelijkheid dat de uitgangsstoffen onder de heersende condities op een andere wijze reageren en andere produkten vormen. Met betrekking tot het thema struktuur-aktivititeitsrelaties begrijpen ze al wel de relatie tussen gelokaliseerde lading en chemische aktiviteit, maar nog niet die tussen gedelokaliseerde lading en aktiviteit. De door mij gekozen chemische context is bedoeld om dit begrijpen te ontwikkelen. De genoemde uitgangsstoffen kunnen namelijk niet alleen met elkaar tot een ether reageren via een nukleofiele substitutie van de tweede orde, maar ook kan een nevenreaktie plaatsvinden, waarbij via het mechanisme van eliminatie een alkeen ontstaat.

De eliminatie-reaktie kan begrepen worden met behulp van factoren die in de chemische struktuur gerepresenteerd kunnen worden door gedelokaliseerde ladingsverschuivingen.
Ik laat zien dat de studenten, die op papier wel degelijk kennis hebben van nevenreakties en van eliminatie (dat hebben ze op het college organische chemie geleerd), deze kennis toch niet funktioneel kunnen toepassen. Zo laat ik zien dat de studenten weliswaar in hun studieboek lezen dat een bepaalde combinatie van uitgangsstoffen tot eliminatie leidt, maar als het er op aan komt dit gegeven in hun besluitvorming negeren. Er is wel kennis, maar die blijkt alleen geschikt voor het reproduceren van correcte antwoorden in de context van een tentamen; niet voor een toepassing in de context van onderzoek. Op cruciale momenten maken studenten keuzes die didactisch alleen te begrijpen zijn door aan te nemen dat ze de thema's niet of onvoldoende begrijpen. Maar in de door mij ontworpen onderwijscontext is het gevolg van hun keuzes niet verwarring, mislukking, of frustratie. De onverwachte chemische verschijnselen die studenten ervaren zijn door mij zodanig gekozen dat de studenten door interpreteren tot dieper inzicht kunnen komen. In dit geval kunnen ze afleiden dat er sprake moet zijn van een nevenreaktie. Zo wordt het begrijpen van dit thema reaktietype uitgebreid.
Mijn bedoeling is dat studenten, in de context van simulatie van onderzoek, zichzelf uiteindelijk theoretische vragen gaan stellen. Wat betreft het thema struktuur-aktiviteitsrelaties betekent dit het formuleren van concrete hypotheses, en het via experimenten onderzoeken, van de factoren die de verhouding ethervorming-eliminatie beïnvloeden. Dat gebeurde in de praktijk echter slechts sporadisch. In plaats daarvan richtten de studenten hun aandacht vooral op het daadwerkelijk maken van de ethers. Zo is synthese als chemische onderzoeksaktiviteit nog te weinig wetenschappelijk van aard.
Ik constateer dan ook dat vervolgonderzoek zich met name op dit probleem zou moeten richten: de overgang van het begrijpen van toepassingsgericht chemisch onderzoeken naar het begrijpen van theoriegericht onderzoek.

In hoofdstuk 8 vat ik mijn onderzoeksresultaten kort samen en bespreek hier ook een probleem dat ik in mijn onderzoek niet kon oplossen: het docentenprobleem. In het practicum Meten & Maken 1, dat gebaseerd is op gedetailleerde voorschriften, is er geen continuïteit met betrekking tot de docenten. Elk jaar, soms zelfs elk half jaar komen nieuwe, onervaren docenten hun 'onderwijstaak' vervullen, om daarna nooit meer in dit onderwijs te participeren. Daarmee werd het voor mij onmogelijk de docenten te betrekken in een cyclus van interpreteren, begrijpen en toepassen. Er bestaat voor de docenten geen noodzaak om op het eigen handelen te reflecteren. Zelfs al zouden ze het doen, dan nog zouden ze hun toegenomen begrijpen niet kunnen toepassen, omdat er voor hen geen nieuwe cyclus is. Dit probleem is bij de gebruikelijke experimenten niet urgent, omdat de docenten net als de studenten een gedetailleerde handleiding krijgen. In de onderwijsvorm simulatie-van-onderzoek daarentegen wordt van de docent verwacht dat hij of zij de ervaringen van de studenten en hun handelen en spreken begrijpt, zodat het gesprek en het experimenteren doelgericht begeleid kan worden. Ik laat zien dat onervaren docenten hiertoe niet zonder meer in staat zijn. Implementatie van onderwijs gebaseerd op simulatie-van-onderzoek zal dan ook consequenties dienen te hebben voor de organisatie van het onderwijs. Deze consequenties en aanpassingen heb ik verder niet onderzocht, omdat dit niet binnen het bestek van mijn onderzoek viel. Mijn doel was het verkrijgen van inzicht in de problematiek van het leren en onderwijzen van organische synthese en, ruimer, organische chemie. Vanuit dat gezichtspunt kan ik mijn onderzoek als geslaagd beschouwen. Aangezien de leerresultaten kwalitatief beter zijn en het onderwijs thematisch en daardoor efficiënter is gestruktureerd, verwacht ik dat de onderwijsvorm simulatie van onderzoek ook in de praktijk uiteindelijk doelmatiger zal zijn. Het 'kookboekprobleem' kan door chemiedidactisch onderzoek worden geanalyseerd. Een oplossing kan worden aangedragen. De implementatie hangt echter samen met de vraag hoe de prioriteiten in het onderwijs worden gelegd door de instanties die daar uiteindelijk voor verantwoordelijk zijn.

Curriculum Vitae

Hanno van Keulen werd op 30 april 1961 geboren in Schiedam. Hij behaalde het diploma VWO in 1979 aan het Meander College te Zwolle. In hetzelfde jaar begon hij met de studie scheikunde aan de Universiteit Utrecht. In 1983 behaalde hij het kandidaatsexamen S1. Hij volgde het bijvak Vaste Stof Chemie en het hoofdvak Fysisch-Organische Chemie, en combineerde dat vanaf 1984 met een aanstelling als assistent op het eerstejaars scheikundepracticum. De ervaringen op dat practicum deden hem besluiten een loopbaan in het scheikunde-onderwijs na te streven. Hij volgde daartoe het bijvak Chemiedidactiek en legde in 1989 het doctoraalexamen af. In hetzelfde jaar volgde hij de tweedefase opleiding tot scheikundeleraar bij het Instituut voor de Leraarsopleiding aan de Universiteit Utrecht.

In 1990 trad hij in dienst van de Faculteit Scheikunde van diezelfde universiteit om bij de Vakgroep Chemiedidactiek het onderzoek te verrichten waarvan in dit proefschrift verslag wordt gedaan. Naast zijn wetenschappelijk onderzoek verrichtte hij diverse onderwijstaken in de Faculteit Scheikunde, zoals op practica voor geologie- en biologiestudenten. Voorts was hij betrokken bij het practicum scheikunde van de Open Universiteit te Heerlen en gaf hij onderwijskundige adviezen aan instelling voor Hoger Beroepsonderwijs. Hij gaf tal van lezingen over zijn werk in binnen- en buitenland, onder andere in Lvov, Los Angeles, en Heidelberg. Zijn wetenschappelijke werk vond internationaal erkenning in zijn benoeming in 1994 tot lid van de Editorial Board van het Amerikaanse tijdschrift Journal for Research in Science Teaching.